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TESTS OF AN URBAN METEOROLOGICAL
POLLUTANT MODEL USING CO VALIDATION
DATA IN THE LOS ANGELES METROPOLITAN
AREA. VOLUME I

Joseph P. Pandolfo, et al

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16. Abstracts The urban boundary-layer model, described in a previous report (Pandolfo et al., 1971), was modified and used in forty test runs. Many of the runs varied the meteorological input about a standard (observed) set. It has, therefore, been demonstrated that an economical, objective, physically consistent, and precisely specified (though with some arbitrary elements) procedure has been achieved for obtaining and predicting the 3-dimensional meteorological fields needed. In several of the runs, the input topography, land-water distribution, and other physical characteristics of the underlying surface was varied. The results demonstrate that ready generalization to other regions can be expected. The modelled region was simulated with relatively coarse (8-mile) grid spacing. This is in contrast to other models which deal with pollutants only, and which are based on 2-mile grid spacing (Sklarew, et al., 1971; Roth et al., 1971). Nonetheless, the temporal and spatial variations of air temperature, humidity, and wind, are simulated with an encouraging degree of realism. Temporal and spatial variations of CO are also simulated fairly realistically, with somewhat less accuracy than in the model described by Roth, et al. (1971), and with accuracy equivalent to that shown by Sklarew, et al. (1971). It is reasonable to expect improved simulation accuracy with the finer horizontal resolution used in these other models, and the performance of such simulations with this model is strongly urged.					
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Meteorological-Pollutant Model
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Metropolitan Area,
Volume I**

by

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May 1973

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1.0 INTRODUCTION

The urban boundary-layer model extensively described in a previous report (Pandolfo, et al., 1971) has been tested with data from Los Angeles, California. The tests were intended to estimate the degree to which observed spatial and temporal variations of meteorological conditions and concentrations of a stable air pollutant could be realistically simulated by the model.

The reader interested in more background discussion of the model is referred to that report. In Section 2.0 of the present report, we do, however, give the set of basic equations again, since these have undergone two major modifications and many minor modifications and corrections. In Section 3.0, the results of several test experiments will be presented. These results are summarized in Section 4.0, and possible steps to improve the performance of the model are suggested. The Appendices give detailed computing formulas used in the computer program, and a discussion and derivation of the modified coordinate system used in the present version of the model. Appendix C, in particular, gives the latest version of the formulas used for radiation calculations in the model computer program. Much of the revision and further development of these formulas carried out since our previous report were not included in the scope of this contract (see Scope of Work), but were carried out under separate sponsorship by one of our associates, Dr. Marshall Atwater. Appendix C is included here to provide the reader with complete documentation of the model in convenient form.

Scope of Work

- 1) The Contractor shall continue the analysis of the simulation results obtained under Contract No. CPA 70-62 and shall modify the previous formulas and computer programs to accept, as a model input an average terrain slope vector for each grid square. This vector shall be used to calculate topographically induced vertical velocities and to modify the calculated values of incident solar radiation at the lower atmospheric interface.

2) The simulation model, as modified under 1) above, shall be applied to approximately six days of meteorological and air quality data selected by the Project Officer for the Los Angeles Basin of California. Evaluation of the model shall be based upon the ability to predict the following conditions:

- a) The spatial and temporal development of the meso-scale meteorological fields that are considered in the model.
- b) The carbon monoxide (CO) concentration field when the model equations for the pollutant field are integrated simultaneously with those predicting the development of the fields of the relevant meteorological variables.
- c) The CO concentration when the observed meteorological fields are treated as specified inputs to the pollutant prediction model.

2.0 THE PLANETARY BOUNDARY LAYER MODEL

2.1 General Description

2.1.1 Designation of Land and Water Grid Points

The set of vertical grid points associated with a grid cell in horizontal space is referred to as a station. Four types of stations can be accommodated by the model. The stations may be characterized by their interfaces and restrictions placed on the subsurface velocity components as follows:

- coastal corner stations have air-water interface and water velocity components identically zero;
- coastal stations also have an air-water interface and the one water velocity component normal to the coastal wall of the grid cell equal to zero;
- water stations have an air-water interface but have no restrictions on the water velocity components directly associated with the station designations;* and
- land stations have a land-air interface and zero subsurface velocity components.

2.1.2 The Terrain-Related Coordinate System

The coordinate system used in the model is based upon a right-handed Cartesian coordinate system with the positive x , y , and z directions taken as east, north, and up, respectively; and with the plane $z = 0$ taken to coincide with some prescribed absolute reference height (e.g., the height of the water surface). The effects of topography are incorporated into the equations by redefining the vertical coordinate to be

$$z = z - \xi(x,y) \quad (1)$$

* Subsurface velocities at water stations might be restricted by the bottom configuration of stations immediately surrounding the water station (see Section 2.2.4.2).

where $\xi(x,y)$ is the elevation of the land or water surface above the reference level, so that the surface $z = 0$ coincides with the interface (i.e. air-land or air-water) (Gerrity, 1967).

The choice of the coordinate system leads to mean velocity advection terms in the prediction equations that may be written in two alternative forms

$$\vec{V} \cdot \nabla X + W \frac{\partial X}{\partial z} = \vec{V} \cdot \nabla_0 X + w \frac{\partial X}{\partial z} \quad (2)$$

where X is the dependent variable and the components of $\nabla_0 X$ are defined in Appendix B. The vertical velocity relative to an absolute reference surface, W , is given by the vertical velocity relative to the terrain, w , plus the terrain induced divergence (see Section 2.2.1 and Appendix B).

In the present version of the model, the absolute reference level $z = 0$ is taken to coincide with the water surface. Thus, $\xi(x,y) = 0$ for stations which contain an air-water interface, viz. coastal, coastal corner, and water stations.

A schematic diagram of this terrain-relative coordinate system superimposed on a lake and surrounding land is presented in Figure 1a. The method of solution for the equations used in the model, i.e. finite-difference techniques, do not resolve the degree of detail shown in Figure 1a but treat the lake and surrounding land as composed of discrete "blocks" centered about a grid point at which values of the dependent variables are determined. The values determined at each grid point are therefore considered as representative of the dynamic or thermodynamic state of the entire block. Figure 1b is a schematic representation of the region shown in Figure 1a as "seen" by the model.

2.1.3 Symbols

The symbols used in this section are defined below with their units (n.d. is nondimensional). Occasionally a symbol, used once, will be defined when used.

- a Surface albedo (n.d.)
- A_i Internal source (sink) for the dependent variable. Units are determined by the i(th) variable.
- $B(x,y)$ Bottom depth for water stations (cm)(see Figure 1a,b).
- c_a Specific heat of air (cal/g/°K).
- c_s Specific heat of subsurface (cal/g/°K).
- c_w Specific heat of water (cal/g/°K).
- $D(x,y)$ Depth at bottom of boundary layer (cm)(see Figure 1a,b).
- E Surface evaporation (g H₂O/cm²/sec).
- f Coriolis parameter (sec⁻¹).
- F Flux of pollutant at surface (g poll/g air/sec).
- F_e Flux of pollutant at elevated level (g poll/g air/sec).
- $F\downarrow(z)$ Downward infrared flux at height z (ly/sec).
- g Gravitational acceleration (cm/sec²).
- h Priestley constant (n.d.).
- $H(x,y)$ Height at top of boundary layer (cm).
- $I(z)$ Incident solar radiation at height z (ly/sec).
- k von Karman constant (n.d.).
- k_1 Kitaigorodsky constant (n.d.).
- K_e Vertical diffusion coefficient for conductivity-diffusivity (cm²/sec).
- K_1 Generalized vertical diffusion coefficient (cm²/sec).
- K_m Vertical diffusion coefficient for momentum (cm²/sec).
- L Latent heat (cal/g).

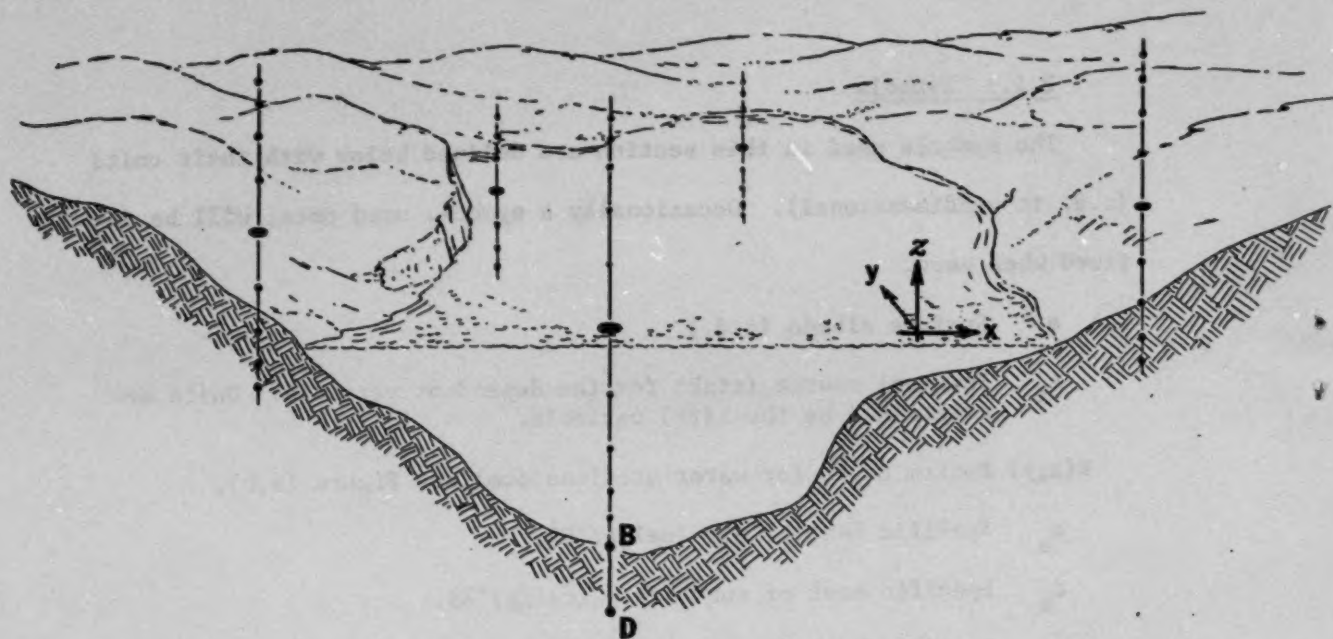


Figure 1a. A schematic diagram of a terrain-relative coordinate system superimposed on a lake and surrounding land.

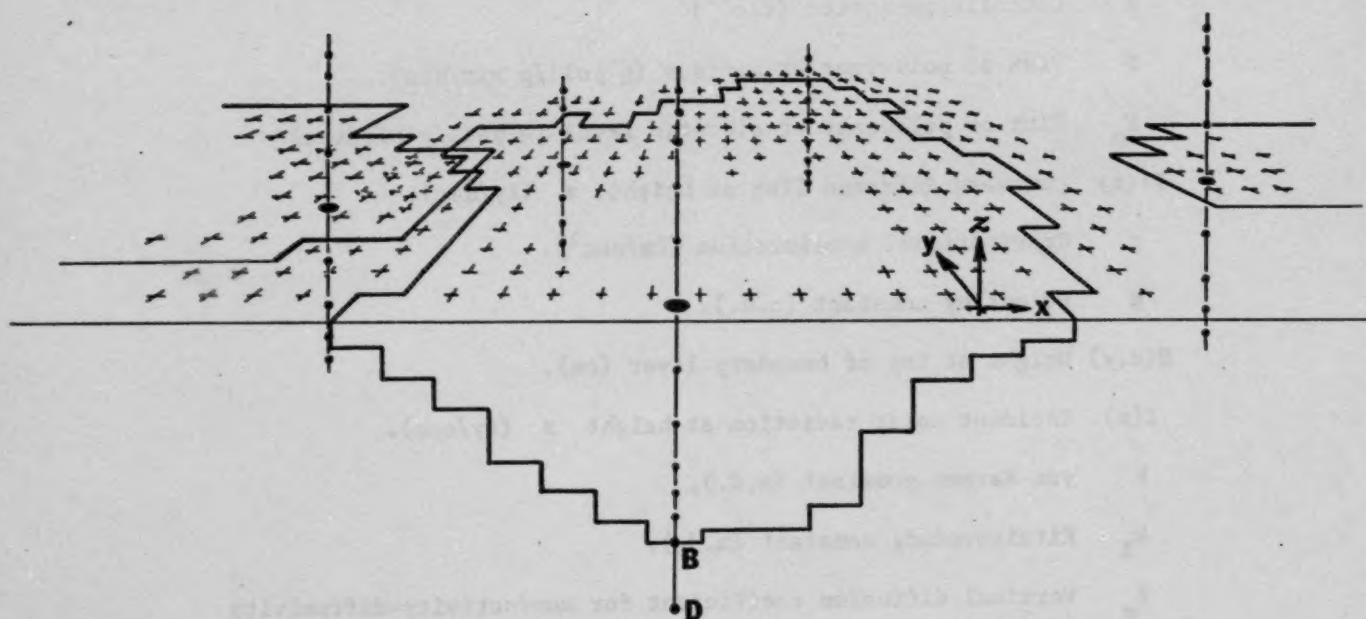


Figure 1b. A schematic diagram of the region shown in Fig. 1a as it might be approximated through the finite-difference techniques used by the model.

M	Halstead moisture parameter, $0 \leq M \leq 1$ (n.d.).
P ₁	Concentration of pollutant 1 ($\mu\text{g}/\text{m}^3$).
P ₂	Concentration of pollutant 2 ($\mu\text{g}/\text{m}^3$).
P _r	Precipitation rate (cm/sec).
q	Specific humidity (g/g).
q _s	Specific humidity at saturation (g/g).
R _s	Incident solar flux at the interface (ly/sec).
R _x	Artificial heat source due to combustion (ly/sec).
Ri	Richardson number (n.d.).
s	Salinity (g/g).
S ₁	Solar radiation source term ($^{\circ}\text{K}/\text{sec}$).
S ₂	Infrared radiation source term ($^{\circ}\text{K}/\text{sec}$).
S _p	Pollutant source term (g poll/g air/sec).
S _w	Vertical gradient of the scalar value of the average orbital velocity in a turbulent wave (sec^{-1}).
t	Time (sec).
T	Temperature ($^{\circ}\text{K}$).
T _r	Temperature of rain ($^{\circ}\text{K}$).
u	Eastward component of velocity (cm/sec).
u _g	Eastward component of geostrophic velocity (cm/sec).
v	Northward component of velocity (cm/sec).
v _g	Northward component of geostrophic velocity (cm/sec).
V _{19.5}	Wind speed at 19.5 m (cm/sec).
$\vec{V}$	Three-dimensional velocity vector (cm/sec).
$\vec{V}_2$	Two-dimensional (horizontal) velocity vector (cm/sec).
w	Upward component of velocity relative to the terrain (cm/sec).
W	Upward component of velocity relative to an absolute reference surface (e.g. mean sea level).

- X_1 Generalized dependent variable.
- z Height relative to the terrain (cm).
- $\bar{z}$ Height relative to an absolute reference surface (cm).
- Z Solar zenith angle (deg).
- $\partial/\partial x_0$ Partial derivative in the x-direction taken along surfaces parallel to the terrain.
- $\partial/\partial y_0$ Partial derivative in the y-direction taken along surfaces parallel to the terrain.
- ∇X_1 Generalized three-dimensional gradient for dependent variable X_1 relative to the absolute reference surface (see Section 3.0).
- $\nabla_0 X_1$ Generalized three-dimensional gradient for dependent variable X_1 relative to the terrain parallel surface (see Section 3.0).
- α Monin-Obukhov constant (n.d.).
- Γ Dry adiabatic lapse rate ($^{\circ}\text{K}/\text{cm}$).
- δ Steepness of characteristic turbulent wave (height to length ratio)(n.d.).
- Δt Time increment (sec).
- η Departure of the water surface elevation from a mean level (cm).
- λ Wavelength of turbulent wave (cm), the roughness height is $\delta = 0$.
- ξ Elevation of the terrain above an absolute reference surface (e.g. mean sea level)(cm).
- ρ Density (g/cm^3).
- σ Stefan-Boltzman constant ($\text{ly}/^{\circ}\text{K}^4/\text{min}$).
- σ_T Density parameter of sea water at atmospheric pressure (g/cm^3).
- τ Transmissivity of radiation (n.d.).

The following subscripts are used to further define variables.

- a Atmosphere.
- g Geostrophic.
- I Interface.

- 0 Relative to the terrain.
- s Subsurface (water or soil).
- w Water.

2.1.4 The General Conservation Equation

The basic equation for the dependent variables takes the form

$$\frac{\partial X_i}{\partial t} + \vec{V} \cdot \nabla_0 X_i = \frac{\partial}{\partial z} \left[K_i(R_i, z) \frac{\partial X_i}{\partial z} \right] + A_i \quad (3)$$

$$i = 1, \dots, 6.$$

The dependent variables include, at most, eastward and northward components of the wind or water currents (u,v), humidity (q), salinity (s), air and subsurface temperature (T), and air pollutants (P₁, P₂). The following sections will describe the specific equations for the atmosphere and subsurface (land or water), and the internal computations of the gradients, exchange coefficients, and source rates.

2.2 The Conservation Equation and Auxiliary Equations

2.2.1 The Atmospheric Layer

The model will include six dependent variables in the atmosphere simultaneously. The equations for the horizontal wind components are written (Pandolfo, 1969) as

$$\frac{\partial u}{\partial t} = -\vec{V} \cdot \nabla_0 u + \frac{\partial}{\partial z} \left[\left(K_m(R_i, z) \right) \frac{\partial u}{\partial z} \right] + f[v - v_g(z)] \quad (4)$$

$$\frac{\partial v}{\partial t} = -\vec{V} \cdot \nabla_0 v + \frac{\partial}{\partial z} \left[\left(K_m(R_i, z) \right) \frac{\partial v}{\partial z} \right] - f[u - u_g(z)] \quad (5)$$

where all symbols have been defined in Section 2.1.1.

$$\frac{\partial T}{\partial t} = -\vec{V} \cdot \nabla_0 T + \frac{\partial}{\partial z} \left[\left(K_e(Ri, z) \right) \frac{\partial T}{\partial z} \right] + \Gamma \frac{\partial K_e}{\partial z} + S_1 + S_2 + WT. \quad (6)$$

The humidity equation is written

$$\frac{\partial q}{\partial t} = -\vec{V} \cdot \nabla_0 q + \frac{\partial}{\partial z} \left[\left(K_e(Ri, z) \right) \frac{\partial q}{\partial z} \right]. \quad (7)$$

The equations for the prediction of pollutants are written

$$\frac{\partial p_i}{\partial t} = -\vec{V} \cdot \nabla_0 p_i + \frac{\partial}{\partial z} \left[\left(K_e(Ri, z) \right) \frac{\partial p_i}{\partial z} \right] + (S_p)_i; \quad (8)$$

$i = 1, 2.$

The formula for the vertical diffusion coefficient and the Richardson numbers are given in Section 2.3.

Geostrophic winds at any height in the layer are computed from the upper boundary value and from the horizontal temperature gradients by use of the integrated form of the thermal wind equation (see, e.g., Hess, 1959, eq. 12.11)

$$u_g(z) = u_g(H) \cdot \frac{T(z)}{T(H)} + \frac{g \cdot T(z)}{f} \int_z^H \frac{1}{T^2} \frac{\partial T}{\partial y} dz, \quad (9)$$

and

$$v_g(z) = v_g(H) \cdot \frac{T(z)}{T(H)} - \frac{g \cdot T(z)}{f} \int_z^H \frac{1}{T^2} \frac{\partial T}{\partial x} dz. \quad (10)$$

The horizontal temperature gradients in eqs. (9) and (10) are relative to the absolute reference surface and are related to the horizontal tempera-

ture gradient relative to the terrain through the equations (see the Appendix):

$$\frac{\partial T}{\partial x} = \frac{\partial T}{\partial x_0} - \frac{\partial T}{\partial z} \frac{\partial \xi}{\partial x} , \quad (11)$$

and

$$\frac{\partial T}{\partial y} = \frac{\partial T}{\partial y_0} - \frac{\partial T}{\partial z} \frac{\partial \xi}{\partial y} . \quad (12)$$

Vertical velocities at any height relative to the terrain are computed from the horizontal velocity gradients by use of the continuity equation for an incompressible fluid

$$w(z) = - \int_0^z \left(\frac{\partial u}{\partial x_0} + \frac{\partial v}{\partial y_0} \right) dz . \quad (13)$$

The vertical velocity relative to the absolute reference surface is computed from the equation

$$W(z) = - \int_0^z \left(\frac{\partial u}{\partial x_0} + \frac{\partial v}{\partial y_0} \right) dz + \left(\frac{\partial \xi}{\partial x} u(z) + \frac{\partial \xi}{\partial y} v(z) \right) . \quad (14)$$

The vertical velocity is, therefore, assumed to be zero at the interface. It is not necessary to specify w at either the upper or lower boundaries (Gerrity, 1967).

2.2.2 The Water Layer*

The time dependent equations for the u and v components of the current are written (Pandolfo, 1969) as

* Recall that in the water layer the absolute reference level $z = 0$ is taken to coincide with the water surface and therefore $z = z$ and $\nabla_0 X_1 = \nabla X_1$.

$$\frac{\partial u}{\partial t} = -\vec{V} \cdot \nabla_0 u + \frac{\partial}{\partial z} \left[\left(K_m(Ri, z) \right) \frac{\partial u}{\partial z} \right] + f[v - v_g(z)] \quad (15)$$

and

$$\frac{\partial v}{\partial t} = -\vec{V} \cdot \nabla_0 v + \frac{\partial}{\partial z} \left[\left(K_m(Ri, z) \right) \frac{\partial v}{\partial z} \right] - f[u - u_g(z)] \quad (16)$$

The temperature in the water layer is computed from Pandolfo (1969)

$$\frac{\partial T}{\partial t} = \vec{V} \cdot \nabla_0 T + \frac{\partial}{\partial z} \left[\left(K_e(Ri, z) \right) \frac{\partial T}{\partial z} \right] + S_1 \quad (17)$$

The salinity is computed from

$$\frac{\partial s}{\partial t} = -\vec{V} \cdot \nabla_0 s + \frac{\partial}{\partial z} \left[\left(K_e(Ri, z) \right) \frac{\partial s}{\partial z} \right] \quad (18)$$

with the diffusion coefficient and Richardson numbers defined in Section 2.3.

The geostrophic currents at any depth are computed from the analogue to the thermal wind equation for the atmosphere, viz.,

$$u_g(z) = u_g(z=0) + \frac{g}{f} \int_{z=0}^z \frac{1}{\rho} \frac{\partial \rho}{\partial y} dz \quad (19)$$

and

$$v_g(z) = -v_g(z=0) + \frac{g}{f} \int_{z=0}^z \frac{1}{\rho} \frac{\partial \rho}{\partial x} dz \quad (20)$$

The horizontal density gradients are computed from the horizontal temperature and salinity gradients based on the relationships presented by Cox et al. (1970).

In the RIGID LID version of the model, the terms $u_g(z=0)$ and $v_g(z=0)$ in eqs. (19) and (20) are prescribed as a function of time. The FREE SURFACE version of the model predicts these values through the equations,

$$u_g(z=0) = -\frac{g}{f} \frac{\partial \eta}{\partial y} \quad (21)$$

and

$$v_g(z=0) = \frac{g}{f} \frac{\partial \eta}{\partial x} \quad (22)$$

Vertical velocities at any depth in the RIGID LID version are computed from the continuity equation

$$W(z) = w(z) = - \int_I^z \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) dz \quad (23)$$

where $W(z=I) = 0$ (the vertical velocity at the air-water interface).

Therefore, W , at the lowest grid level in the water, is not prescribed but predicted through eq. (23) and is physically analogous to an open bottom boundary in the water layer capable of absorbing gravity waves.

In the FREE SURFACE version, the vertical velocities at any depth are computed by integration of the continuity equation which yields the result

$$W(z) = w(z) = - \int_B^z \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) dz \quad (24)$$

where use has been made of the fact that $W(z=B) = 0$. The vertical velocity at the interface computed from eq. (24) is used to predict the water surface elevation through the equation

$$\frac{\partial \eta}{\partial t} = W(z=I) \quad (25)$$

Equations (24) and (25) lead to a free water surface elevation and to the introduction of undamped gravity waves at the water-air interface.

2.2.3 Dependent Variables in the Soil

Temperature is the only time dependent variable in the soil and is governed by the equation

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left(K_e(z) \frac{\partial T}{\partial z} \right), \quad (26)$$

where $K_e(z)$ is the thermal diffusivity, which is specified as a function of height. No other variables are simulated in the soil.

2.2.4 Boundary and Interface Conditions

2.2.4.1 Atmosphere

The dependent variables in the atmospheric layer are specified at the upper boundary. The velocity field must be nondivergent but can be prescribed as a function of time at the upper boundary. At lateral inflow boundaries, the gradients of the dependent variables are prescribed rather than calculated in the program.

2.2.4.2 Water

The temperature, salinity, and two pollutants are fixed at the bottom water boundary. When the model includes land underlying the water, the vertical temperature profile is specified, and the salinity and pollutants are taken identically zero. The horizontal velocities are subject to kinematic boundary conditions with slip allowed at lateral boundaries. These conditions are expressed as follows for each of the four types of water stations:

$$\left. \begin{array}{l} u_w(z) = 0 \\ v_w(z) = 0 \end{array} \right\} ; D(x,y) \leq z \leq 0 \quad \left. \begin{array}{l} \text{Coastal corner station} \\ \end{array} \right\} \quad (27a)$$

$$\left. \begin{array}{l} u_w(z) = 0 \\ v_w(z) = 0 \end{array} \right\} ; D(x,y) \leq z \leq B(x,y) \quad \left. \begin{array}{l} \text{For a coastal station} \\ \text{which is oriented parallel} \\ \text{to the latitude lines} \\ \text{(east-west coast)} \end{array} \right\} \quad (27b)$$

$$\left. \begin{aligned} u_w(z) &= 0 ; D(x,y) \leq z \leq 0 \\ v_w(z) &= 0 ; D(x,y) \leq z \leq B(x,y) \end{aligned} \right\} \begin{array}{l} \text{For a coastal station} \\ \text{which is oriented perpen-} \\ \text{dicular to the latitude} \\ \text{lines (north-south coast)} \end{array} \quad (27c)$$

$$\left. \begin{aligned} u_w(z) &= 0 ; D(x,y) \leq z \leq B'_{NS} \\ v_w(z) &= 0 ; D(x,y) \leq z \leq B'_{EW} \end{aligned} \right\} \begin{array}{l} \text{For a water station} \end{array} \quad (27d)$$

where B'_{NS} is the bottom depth of the shallower of two stations immediately north or south of the water station, and B'_{EW} is the bottom depth of the shallower of two stations immediately east or west of the water station. Thus, B'_{NS} and B'_{EW} depend on the system of grid points to be chosen. These definitions imply an additional constraint on a water station: that a water station must always be surrounded by stations that have air-water interfaces (i.e. coastal corner, coastal, or another water station). By accounting for the bottom topography of the immediately adjacent east-west and north-south stations, the model is able to apply the proper kinematic and slip boundary conditions for a variable-depth water basin.

Both versions of the model can accommodate open lateral water boundaries (therefore, the model can handle inflows and outflows to a lake basin). The use of this type of boundary requires the gradients of the dependent variables used in the prediction equations at an inflow boundary station to be specified rather than the calculated gradients. An additional requirement is the specification of the water surface elevation outside all open lateral water boundaries. This condition allows the water velocities at open boundaries to be determined by the model.

2.2.4.3 The air-water-soil interface

Values of the dependent variables are obtained at the interface and are highly dependent on the nature of the subsurface (water or soil). In the case of water, several equation parameters are computed, while for soil,

they are specified. These parameters include albedo, a moisture parameter, specific heat of the subsurface material, density of the subsurface material, and the roughness height.

It is assumed that there are no discontinuities in velocity or temperature. This leads to the interface velocity condition over water given by

$$(\vec{V}_I)_a = (\vec{V}_I)_w \quad (28)$$

For a soil subsurface, a no-slip condition is used, i.e. $\vec{V}_2 = \vec{0}$, at $z = z_0$; i.e., the velocity vanishes at some height above the interface. For a water surface, the additional condition imposed is that the horizontal shearing stress is continuous,

$$\rho_a \left(K_m \frac{\partial \vec{V}_2}{\partial z} \right)_a = \rho_w \left(K_m \frac{\partial \vec{V}_2}{\partial z} \right)_w \quad (29)$$

The interface specific humidity q_I is computed from

$$q_I = M(q_s) + (1 - M) q_1 \quad (30)$$

where q_1 is the humidity at the first atmospheric grid level. The parameter is 1 for water and 0 for dry soil. For moist soil cases, M takes on intermediate fractional values. Halstead et al. (1957) discussed the empirical evaluation of M when it falls into this intermediate range.

The evaporation, E , is computed from

$$E = \rho_a K_{e_a} \frac{\partial q}{\partial z} \quad (31)$$

The interface salinity, when required, is computed from

$$s = 1 - \frac{E - P_r}{\rho_w K_{e_w} \frac{\partial T}{\partial z}} \quad (32)$$

The interface temperature is computed by an iterative solution to the heat balance equation (see e.g., Pandolfo, 1969) by

$$0 = R_s + F(0) - [L \cdot E](T_I) - \sigma T_I^4 - \rho_a c_a K_{e_a} \left[\left(\frac{\partial T}{\partial z} \right)_+ + \Gamma \right] (T_I) \\ - \rho_s c_s K_{e_s} \left(\frac{\partial T}{\partial z} \right)_- (T_I) + c_w \rho_w P_r (T_r - T_I) + R_x \quad (33)$$

where the subscripts on the temperature gradients indicate derivatives taken on the atmospheric side of the interface (+), or the water/soil side of the interface (-). The assumption that the temperature is continuous at the interface is applied in the calculation of the individual terms in the balance equation.

The solar radiation term is computed from

$$R_s = (1 - a) I(0) - \tau_s I(0) \quad (34)$$

with τ_s the transmission of solar energy through the water interface (zero for a soil interface) and $I(0)$ the solar energy at the surface. The solar energy reaching the surface is computed by methods described in a forthcoming report (see Section 2.4). The albedo is specified when the subsurface is soil and is computed from

$$a = - .0139 + .0467 \tan Z \quad (35)$$

$a \geq .03$ when the subsurface is water (Sverdrup et al., 1942).

The amount of solar radiation absorbed by the water is used to complete the source term for solar radiation in the water layer. The source term is

computed from Hess (1959) as

$$S_1 = \frac{1}{\rho_w c_w} \frac{\partial I_a}{\partial z} \quad (36)$$

According to Beer's law, the intensity of solar radiation at any level is given by

$$I(z) = I(0) e^{-\kappa_w \Delta z \sec Z}, \quad (z < 0) \quad (37)$$

where all radiation and absorption terms have been integrated over the solar spectrum. Because of selective extinction in the water, the value of κ_w is computed as an empirical function of depth from observations.

The absorption coefficients are computed or linearly interpolated from data for the oceans, presented by Sverdrup et al. (1942) and Kondrat'yev (1969), and are shown in Table 1. For Lake Ontario, an empirical relation

TABLE 1
Extinction Coefficients in the Ocean

Depth	κ_w
< 2 m	$\kappa = 1.034 - .5698 \ln z$
2 m	.6370
5 m	.3510
10 m	.2350
20 m	.1650
50 m	.1160
100 m	.0977

based on data presented by Beeton (1962) is given by

$$\kappa_w = 0.524 - 0.014z + .0034z^2 \quad (38)$$

where z is the depth in meters. This formula may turn out to be more generally representative of inland water than are the oceanic tabular values.

The infrared radiation flux received at the interface is calculated by methods described in a forthcoming report (see Section 2.4).

The seventh term includes the effect of rain on the heat balance temperature. The temperature of the rain is assumed to equal the height average of wet bulb temperature in the layer of air near the surface. While the thickness of the layer appears to be realistic for the tropical oceans, the validity of this thickness has not been tested in other regions.

The final term is an artificial heat source (heat added per unit area per unit time) due to the activities of man by combustion of fossil fuels.

When the subsurface is soil, the albedo, the density, the specific heat, the thermal diffusivity, and the moisture parameters are specified. They are computed for water.

The value of pollutant concentration at the interface is calculated from a flux value using the formula

$$P_i(z_i, t) = P_i(z_{i+1}, t) - \frac{F \Delta z}{K_e(z_{i+1}, t)}, \quad (39)$$

where $i = 1, 2$ and F is the surface flux of pollutant as given in the inventory. Note that $K_e(z_{i+1}, t)$ and $P_i(z_{i+1}, t)$ are calculated by the model.

The flux of pollutant into the atmosphere is not restricted to a source at the ground and can occur at various elevations. Therefore, the model has been developed to include elevated sources. The emission strengths from the source inventory are divided and assigned, according to the nature of the source, to points on the vertical grid. The strength at the inter-

face is set by eq. (39). At the higher elevations, the pollutant is assumed to be instantaneously mixed in the layer that is bounded by the midpoints of the layers adjacent to the grid level. This results in a source term

$$S_p = \frac{F_e}{\rho \Delta z} \quad (40)$$

2.3 Vertical Diffusion Coefficients

The vertical diffusion coefficients are internally computed in the model as a function of the vertical gradients of wind, humidity, and temperature. The method has been previously described by Pandolfo (1969) and Pandolfo and Brown (1970).

When the subsurface is water, the formulas for the Richardson number and vertical diffusion coefficients are modified to include mixing length variations due to the presence of a "mean turbulent wave" at the interface. The formulations used here are based on work by Kitaigorodsky (1961). The parameters needed include δ , the wave steepness (height to length ratio), and λ , the wavelength. The wavelength is found using the wind speed at 19.5 m (Pierson, 1964) by

$$\lambda = 28.03 \times 10^{-4} (V_{19.5})^2 \quad (41)$$

Pierson also suggested that a constant steepness is appropriate for many applications in "fully developed" seas. The value 0.055 is used in the model when "fully developed" waves are indicated and is zero when the surface is soil.

Note that the modelling formulas shown are for "fully developed" seas and are applied when over water to bring the parameterized wave state into

immediate and complete adjustment with the low level wind. The method needs revision for the simulation of duration-limited or fetch-limited cases. For example, the wavelength could be reduced by a given fraction.

The relevant wave property used in the calculation of the Richardson numbers and exchange coefficients is the vertical gradient of the scalar value of the average orbital velocity in the turbulent wave given by

$$S_w = g^{\frac{1}{2}} \delta \left(\frac{\lambda}{2\pi} \right)^{-\frac{1}{2}} e^{-z2\pi/\lambda} \quad (42)$$

In essence, this velocity shear, S_w , is added to the shear of the mean velocity when calculating Richardson numbers and vertical diffusion coefficients.

Richardson numbers are not computed at the first grid levels adjacent to the interface in either the atmospheric or water layers for computational convenience. This does not lead to unrealistic results for a shallow enough grid layer. Therefore, the Richardson numbers are assumed to be zero at these grid levels in the following computations for the water case.

Whenever the subsurface is land, the term S_w is zero.

The Richardson numbers in the atmosphere are computed as a function of height from

$$Ri = \frac{g}{T} \left[\frac{\partial T}{\partial z} + \Gamma + .61\bar{T} \left(\frac{\partial q}{\partial z} \right) \right] \left(\left| \frac{\partial \vec{V}_2}{\partial z} \right| + S_w \right)^{-2} \quad (43)$$

where $Ri \leq 1/|a|$. The Richardson numbers in water are computed from

$$Ri = - \frac{g}{\rho_w} \left(\frac{\partial \rho_w}{\partial z} \right) \left(\left| \frac{\partial \vec{V}_2}{\partial z} \right| + S_w \right)^{-2} \quad (44)$$

The density gradient ($\partial\rho_w/\partial z$) is computed (e.g., Sverdrup et al., 1942) from

$$\frac{\partial\rho_w}{\partial z} = 10^{-3} \frac{\partial\sigma_T}{\partial z} = 10^{-3} \left(\frac{\partial\sigma_T}{\partial T} \frac{\partial T}{\partial z} + \frac{\partial\sigma_T}{\partial s} \frac{\partial s}{\partial z} \right), \quad (45)$$

where the values of $\partial\sigma_T/\partial T$ and $\partial\sigma_T/\partial s$ are obtained by differentiation of an empirically obtained formula for σ_T given by Cox et al. (1970).

The exchange coefficient formulas for the atmospheric layer are consistent with the profile formulas discussed by Pandolfo (1966), except that the shear S_w is added to the shear $|\partial\vec{V}_2/\partial z|$.

Thus, for stable conditions, the eddy viscosity K_m is given by

$$K_m = k^2 \left(z + \frac{\delta\lambda}{2} \right)^2 \left(\left| \frac{\partial\vec{V}_2}{\partial z} \right| + S_w \right) \left(1 + \alpha Ri \right)^2, \quad (46)$$

$$Ri \geq 0,$$

where $k = 0.4$; and the eddy conductivity-diffusivity is assumed to be

$$K_e = K_m. \quad (47)$$

For lapse forced convection conditions, the formulas are

$$K_m = k^2 \left(z + \frac{\delta\lambda}{2} \right)^2 \left(\left| \frac{\partial\vec{V}_2}{\partial z} \right| + S_w \right) \left(1 - \alpha Ri \right)^{-2}, \quad (48)$$

and

$$K_e = K_m \left(1 - \alpha Ri \right)^{-1}, \quad (49)$$

where $-0.048 < Ri < 0$. For lapse free convection conditions, i.e. for $Ri \leq -0.048$, the formulas are

$$K_e = h \left(z + \frac{\delta\lambda}{2} \right)^2 \left| \frac{g}{T} \left(\frac{\partial T}{\partial z} + \Gamma + .61\bar{T} \left(\frac{\partial q}{\partial z} \right) \right) \right|^{1/2} \quad (50)$$

and

$$K_m = K_e \left(\frac{3}{C} \right)^{-1/2} |Ri|^{-1/6}, \quad (51)$$

where

$$C = 3k^{4/3} h^{-2/3}, \quad (52)$$

and h is the Priestley constant. See Pandolfo (1966) for more detail on the formulas and constants used in lapse conditions.

Computed values for the eddy exchange coefficients for extreme stability are meaningless whenever they fall below estimates for minimum values in the atmospheric boundary layer (Pandolfo, 1969). The minimum values used for the atmosphere are:

$$10^4 \leq K_{e,m} \leq 10^7 \quad z \geq 100 \text{ m},$$

$$\Lambda \leq K_{e,m} \leq 10^7 \quad z < 100 \text{ m}.$$

where $\Lambda = \lambda^2 = z_0^2$ for a land subsurface or $\Lambda = (H_{1/3})^2$ for water subsurface. Here z_0 is the roughness height, and $H_{1/3}$ is the 1/3 highest wave (see eq. 67).

The exchange coefficient formulas used for the oceanic layer are the modified Rossby-Montgomery formulas (after Kitaigorodsky, 1961) for stable stratification:

$$K_m = k_1^2 \left(\left| \frac{\partial \vec{v}_2}{\partial z} \right| + S_w \right) \left(1 + 10 Ri \right)^{-1/2}, \quad (53)$$

and

$$K_e = k_1^2 \left(\left| \frac{\partial \vec{v}_2}{\partial z} \right| + S_w \right) \left(1 + \frac{10}{3} Ri \right)^{-3/2}, \quad (54)$$

where $Ri \geq 0$. For these formulas, Kitaigorodsky assigned an estimated value of $k_1^2 = 0.02$. For lapse forced convection conditions ($-0.048 <$

$Ri < 0$), the formulas are given by eqs. (48) and (49) with the Kitaigorodsky, constant (k_1), replacing the von Karman constant (k).

For unstable stratification in the oceanic layer, the exchange coefficients are given by

$$K_e = h \left(z + \frac{\delta\lambda}{2} \right)^2 \left| g \frac{\partial \ln \rho}{\partial z} \right|^{1/2} \quad (55)$$

and

$$K_m = K_e \left(\frac{3}{C} \right)^{-1/2} |Ri|^{-1/6}, \quad (56)$$

where $Ri \leq -0.048$, and

$$C = 3k^{4/3} h^{-2/3} \quad (57)$$

Limiting values of the water exchange coefficient for stable conditions, based on values that correspond to molecular viscosity, and conductivity-diffusivity, are

$$K_m \geq 0.14 \text{ cm}^2/\text{sec}$$

$$K_e \geq 0.0014 \text{ cm}^2/\text{sec},$$

respectively.

2.4 Solar and Infrared Radiation

A discussion of the methods for obtaining the solar and infrared radiation source terms in the model will be presented in Appendix C, written by Dr. Atwater, under separate sponsorship.

2.5 Computer Considerations

The model program is written to take any arbitrary number of horizontal grid points in any rectangular array without further reprogramming (see Vol. II for further detail). The practical restriction on the horizontal resolution then becomes the duration (and cost) of a single simulation run. With the grid here used (8-mile horizontal grid mesh) we ran 40 test runs with the hydrostatic model and several test runs with the non-hydrostatic model. It was realized that the 8-mile grid resolution would fail to capture smaller horizontal scales which contained important variability in the emission source patterns, but it was decided that at this state of development it was preferable to gain experience with many variations of the meteorological input. An alternative course which was rejected would have allowed, within the same computer budget, something like three test runs with the 2-mile horizontal grid mesh more commonly used in pollutant models. Still another alternative is possible because of the program option which allows the meteorological variables to be input. This would run the full model (meteorological plus conservative pollutants) on a relatively coarse horizontal grid (say, with 8-mile mesh spacing), and subsequently run a fine resolution (say, with 2-mile grid mesh) simulation, with the meteorological solutions of the first run input and interpolated to the fine grid.

We have estimated the time and costs required to run the full model (meteorological plus conservative pollutants) over a 24-hour simulation period on the 2x2 mile horizontal grid. This would cover the Los Angeles region with a grid network consisting of 25x25 (horizontal) x15 (vertical) grid points. Our experience with the simulations run thus far yields a running time of about 2 seconds (IBM 360-65) per mesh point for simulation over a 24-hour period. For this computer system, therefore, a 24-hour simu-

lation would take approximately five hours at a cost of about \$1,000*.

Relative time on other systems available in the Hartford area are 1/3

(IBM 370/155; UNIVAC 1108) and 1/33 (CDC 7600). Relative costs* on these

systems are 0.58 (IBM 370/155), 0.85 (UNIVAC 1108); and .41 (CDC 7600).

* These costs are based on off-shift rates on systems available to CEM locally in the Hartford area.

3.0 TEST SIMULATIONS WITH THE BOUNDARY LAYER MODEL

3.1 The Input Data

3.1.1 The Modelled Region

The decision was made early in the course of the work to begin with experiments performed on a relatively coarse horizontal grid for reasons of economy. Also, as implied by eqs. (9) and (10) (Section 2.2.1), the hydrostatic approximation is applied in the present version of the model; while this approximation should be valid for wind systems resolved on horizontal grids with mesh spacing of the order of 10 km, its validity becomes questionable with much finer resolution. The computer program for a non-hydrostatic version of the model has been checked out recently, but was not available at the time of the work reported here. The modelled region was chosen to cover a smaller area than that used by Roth et al. (1971), with a horizontal grid cell dimension of 8 miles, rather than their 2 miles. The two grid arrays, and their location in the Los Angeles region, are shown in Figure 2.

The grid chosen resulted in the distribution of land and water grid cells shown in Figure 3. The distinction between different types of water grid cells is used in the application of barrier boundary conditions in the prediction of subsurface flow. Of greater relevance in this project is the basic distinction between land and water grid cells, and its effect on meteorological conditions in the region. This will be seen later during the discussion of the results of one experiment in which all grid cells in the modelled region were treated as if they were land cells. It should be noted that the greatest ambiguity in the definition of a grid cell type arose in the case of grid cells 3,1 and 5,4.

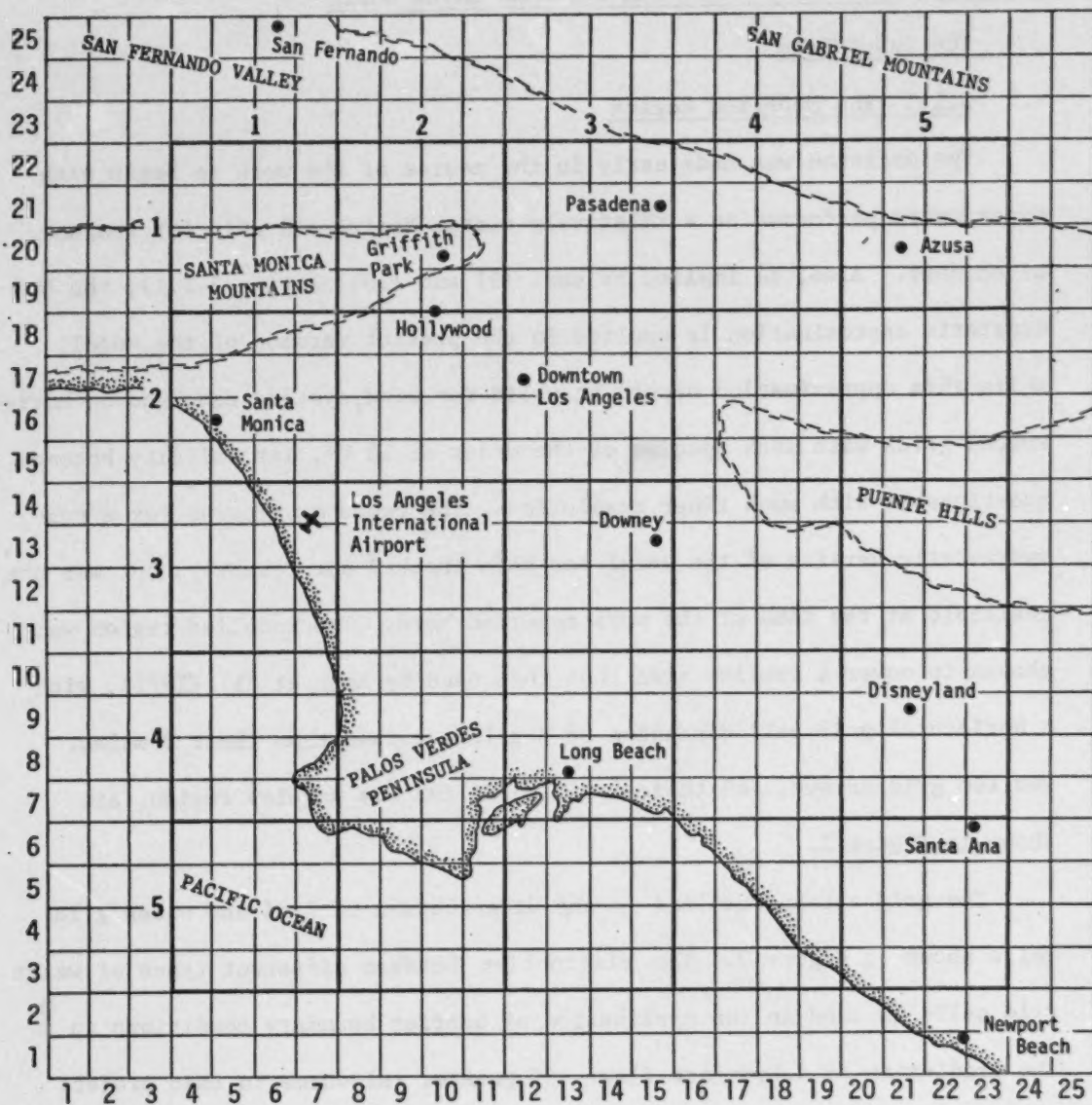
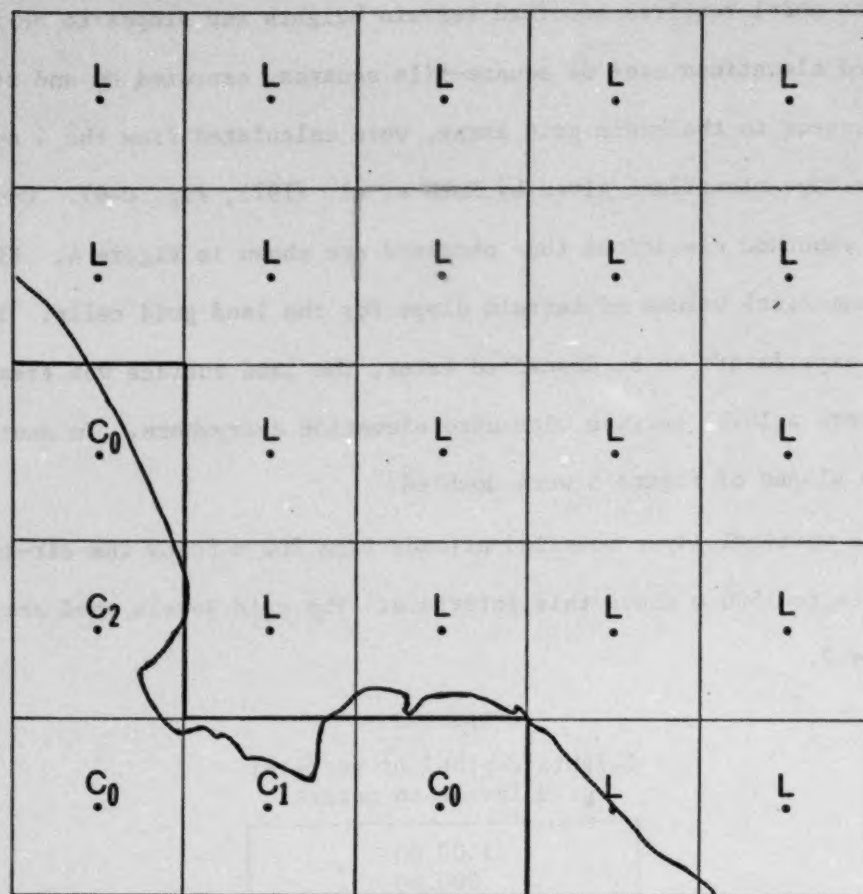


Figure 2. The locations of the horizontal grid used by Roth et al. (1971) and of the coarser, smaller area grid used in this report are shown.



← 12.87 km →
← 8 mi →

Key

- L Land cell.
- C₀ Coastal cell containing barrier walls to both N-S and E-W subsurface flow.
- C₁ Coastal cell containing barrier walls to N-S subsurface flow.
- C₂ Coastal cell containing barrier walls to E-W subsurface flow.

Figure 3. Modelled distribution of land and water grid cells in the region.

The model requires smoothed terrain heights and slopes to be input. Averaged elevations over 64 square-mile squares, centered on and staggered with respect to the basic grid array, were calculated from the 4 square-mile average elevations given by Roth et al. (1971, Fig. C-9). Contours of the smoothed elevations thus obtained are shown in Figure 4. Figure 5 shows numerical values of terrain slope for the land grid cells. In one of the experiments to be described later, the land surface was treated as if it were a level surface with zero elevation everywhere. In another, the terrain slopes of Figure 5 were doubled.

The vertical layer modelled extends from 200 m below the air-soil(water) interface to 1500 m above this interface. The grid levels used are listed in Table 2.

TABLE 2
Heights(depths) of vertical
grid levels in meters

1500.00
900.00
650.00
450.00
300.00
150.00
75.00
25.00
4.00
0.00
- 0.05
- 0.10
- 0.15
- 0.20
- 1.00
- 10.00
- 50.00
-100.00
-200.00

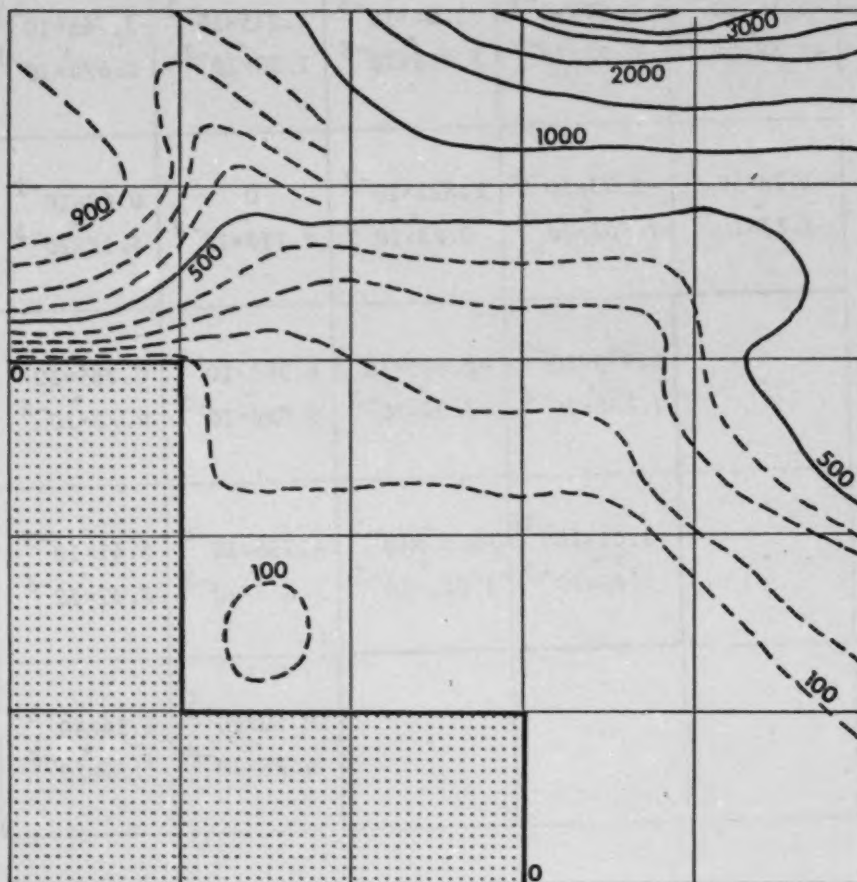


Figure 4. Contours (labeled in feet) of smoothed elevation used to calculate terrain slopes input to the model.

-4.18×10^{-3} -2.58×10^{-3}	4.97×10^{-3} 0.77×10^{-2}	1.04×10^{-3} 3.775×10^{-2}	1.215×10^{-2} 1.20×10^{-1}	-2.745×10^{-3} 0.575×10^{-1}
-1.78×10^{-2} 2.33×10^{-2}	-2.77×10^{-3} 1.005×10^{-2}	1.825×10^{-3} 0.98×10^{-2}	0 0.715×10^{-2}	0.63×10^{-2} 3.17×10^{-3}
.	2.985×10^{-3} 1.705×10^{-3}	-2.605×10^{-4} 3.08×10^{-3}	4.995×10^{-3} 4.095×10^{-3}	0.785×10^{-2} 0.78×10^{-2}
.	1.61×10^{-3} 1.80×10^{-3}	-0.57×10^{-3} 1.655×10^{-3}	4.735×10^{-4} 1.375×10^{-3}	3.41×10^{-3} 3.41×10^{-3}
.	.	.	0.52×10^{-3} 4.26×10^{-4}	1.16×10^{-3} 1.16×10^{-3}

Figure 5. Values of terrain slope calculated from smoothed elevation, where the upper values are the eastward component of the slope ($\partial \xi / \partial x$); and the lower values (italic) are the northward components of the slope ($\partial \xi / \partial y$).

3.1.2 Physical Parameters of the Interface

A brief discussion of the considerations involved in prescribing these parameters is given in Pandolfo et al. (1971, Section 3.2). In the Los Angeles experiments, the values used in the base run (Run 37) are shown in Table 3.

TABLE 3
Physical parameters of the interface

Parameter	Land	Water
Albedo (n.d.)	.20	*
Soil heat conductivity (cal/cm sec °K)	.005	*
Soil specific heat (cal/gm °K)	.26	1.0
Soil density (gm/cm ³)	2.00	1.0
Roughness height (cm)	100.00	*
Moisture Parameter (n.d.)	0.1**, 0.0	1.0
Artificial heat source (mly/sec)	0.0	0.0

* These values are internally computed for water grid squares.

** This value was used for grid squares 2,1 and 2,2, which cover the seaward slopes of the Santa Monica Mountains.

In one of the experiments to be described later, the moisture parameter was changed to 0.2 at all land stations.

3.1.3 Initial fields

Typically, the meteorological observations available for simulations of this kind consist of a single vertical sounding, or at best, a small number of such soundings, in a much denser net of surface observations. The initial fields of meteorological variables are, therefore, constructed in the computer program from input vertical profiles at an arbitrarily specified horizontal grid point (chosen to coincide as closely as possible with the location of the observed sounding); and horizontal gradients (in

terrain parallel surfaces) of these variables at selected heights above the terrain. The construction is by linear extrapolation in the horizontal. The program is written so that it is also possible to input meteorological variables in this manner at other times during the period of simulation, and to circumvent the model prediction of wind, or temperature, or humidity, or any combination of these three variables.

In the Los Angeles observations, temperature and humidity profiles were measured at Los Angeles International Airport twice daily at 14GMT and 18GMT. Therefore, 14GMT (06 PST), 29 September 1969, was chosen as the initial time for the experiments. The nearest wind soundings were measured twice daily at 00GMT and 12GMT at San Nicolas Island and Vandenberg Air Force Base, well outside the modelled area. Hourly surface weather observations are available at four locations within the modelled region (viz., USAS, Los Alamitos (NTB); Daugherty Field, Long Beach (LONB); Burbank (BURK); and Los Angeles International Airport (LAX)). The location of these stations within the modelled region is shown in Figure 6.

The base run (Run 37) used vertical profiles of temperature and humidity derived from the LAX sounding at 14GMT, 29 September 1969. These are shown in Table 4, and were input at grid point 3,2. Horizontal gradients of temperature and humidity at the surface were obtained by fitting a plane to the surface observations at the four stations shown in Figure 6, and observations at two additional stations outside the region (viz., Van Nuys, California, and Ontario, California) and are shown in Table 5.

The large-scale vorticity of horizontal wind near the surface was obtained from measured winds in the same way, i.e. by plane fit to the observations, and is also shown in Table 5. The divergence of the initial wind

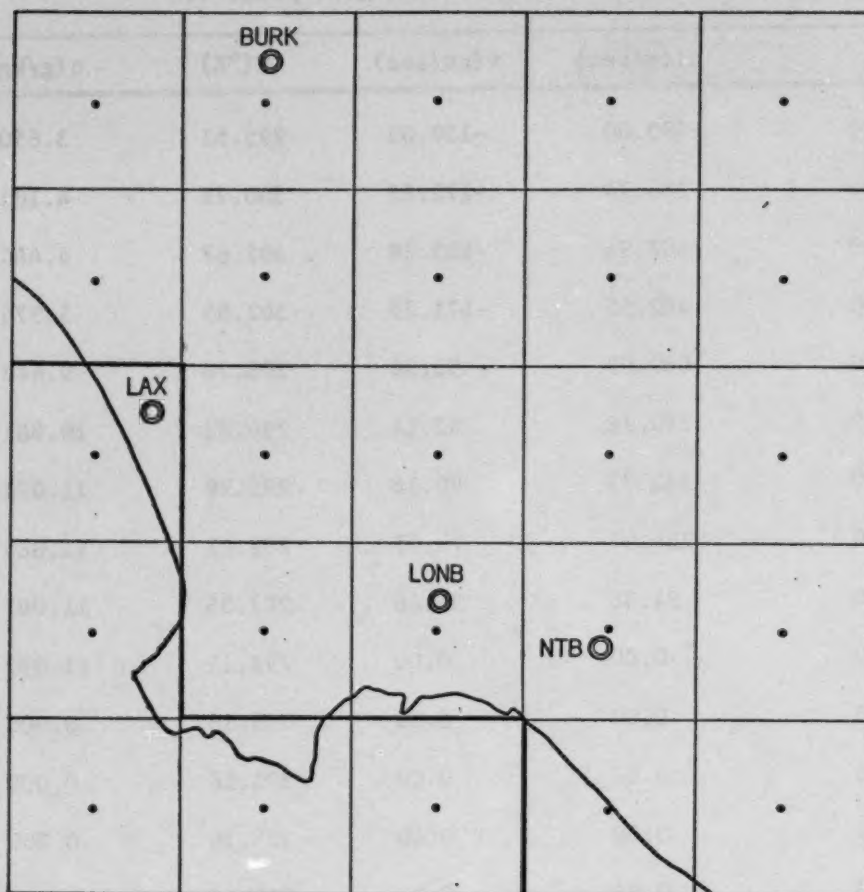


Figure 6. Location of surface weather observing stations in modelled region.

TABLE 4
Initial vertical profiles of meteorological variables
used in the base run at grid point 3,2

z(m)	u(cm/sec)	v(cm/sec)	T(°K)	q(g/kg)
1500.00	490.00	-150.00	295.51	3.650
900.00	286.74	-171.83	300.71	4.101
650.00	402.94	-185.28	302.67	4.486
450.00	482.55	-171.29	302.55	5.974
300.00	680.09	- 58.34	298.78	9.442
150.00	740.18	42.14	296.82	10.881
75.00	582.33	90.18	295.29	11.071
25.00	254.97	79.97	292.91	11.085
4.00	94.36	34.46	292.35	11.087
0.00	0.00	0.00	291.11	11.087
- 0.05	0.00	0.00	303.16	0.000
- 0.10	0.00	0.00	303.16	0.000
- 0.15	0.00	0.00	303.16	0.000
- 0.20	0.00	0.00	303.16	0.000
- 1.00	0.00	0.00	289.98	0.000
- 10.00	0.00	0.00	286.86	0.000
- 50.00	0.00	0.00	284.66	0.000
-100.00	0.00	0.00	282.66	0.000
-200.00	0.00	0.00	281.56	0.000

TABLE 5

Horizontal gradients of meteorological variables input to the base run.

$z(m)$	$\frac{\partial u}{\partial x}(\text{sec}^{-1})$	$\frac{\partial u}{\partial y}(\text{sec}^{-1})$	$\frac{\partial v}{\partial x}(\text{sec}^{-1})$	$\frac{\partial v}{\partial y}(\text{sec}^{-1})$	$\frac{\partial T}{\partial x}(\text{°cm}^{-1})$	$\frac{\partial T}{\partial y}(\text{°cm}^{-1})$	$\frac{\partial q}{\partial x}^*$	$\frac{\partial q}{\partial y}^*$
1500	0	$.48867 \times 10^{-4}$	$.22654 \times 10^{-5}$	0	0	0	$-.71197 \times 10^{-7}$	$-.16181 \times 10^{-6}$
900	0	$.15534 \times 10^{-4}$	$.61489 \times 10^{-5}$	0	X	X	$-.19094 \times 10^{-6}$	$-.48867 \times 10^{-6}$
650	X	X	X	X	0	0	X	X
450	0	$.37217 \times 10^{-4}$	$.14240 \times 10^{-4}$	0	X	X	$-.20388 \times 10^{-6}$	$-.50485 \times 10^{-6}$
300	0	$-.38835 \times 10^{-5}$	$-.16829 \times 10^{-4}$	0	X	X	$-.19741 \times 10^{-6}$	$-.49515 \times 10^{-6}$
75	0	$-.35599 \times 10^{-4}$	$-.18770 \times 10^{-4}$	0	X	X	$-.17799 \times 10^{-6}$	$-.50809 \times 10^{-6}$
2	0	$-.27710 \times 10^{-4}$	$.18854 \times 10^{-4}$	0	$.12618 \times 10^{-6}$	$.44229 \times 10^{-6}$	$-.32151 \times 10^{-6}$	$-.70550 \times 10^{-6}$
0	0	0	0	0	0	0	0	0
-200	0	0	0	0	0	0	0	0

* Units in $g(\text{kg}/\text{cm})$.

field was set everywhere at 0 in the base run. The vertical profile of wind for the base run was taken from the output of an auxiliary run which had its initial profile derived from the 12GMT average of the San Nicolas and Vandenberg RAWINS above the surface layer and which was run through a 24-hour simulation period. The initial vertical wind profile for this run, derived from the RAWINS, is shown in Table 6.

TABLE 6

Vertical profiles of wind derived from the San Nicolas-Vandenberg RAWINS and surface observations (in cm/sec)

z(m)	12GMT/29 Sep.		00GMT/30 Sep.		12GMT/30 Sep.	
	u	v	u	v	u	v
1500.0	490.0	-150.0	20.0	- 50.0	350.0	-205.0
900.0	415.0	-325.0	145.0	- 65.0	310.0	- 22.0
650.0	255.0	-230.0	250.0	-160.0	210.0	-105.0
450.0	110.0	-135.0	310.0	-150.0	135.0	- 15.0
300.0	230.0	0.0	320.0	0.0	85.0	- 10.0
150.0	330.0	110.0	335.0	130.0	35.0	- 10.0
75.0	375.0	155.0	345.0	205.0	10.0	- 5.0
25.0	409.0	189.0	348.0	287.0	90.0	55.0
4.0	420.0	210.0	350.0	305.0	165.0	95.0

The values of initial horizontal gradients at heights above the surface layer must be guessed, because only one vertical sounding was available within the modelled region. For the base run, the vorticity of the wind at the upper boundary (1500 m above the terrain) was derived from the observed average profile by assuming that the winds aloft were homogeneous in planes parallel to sea level. The humidity at the upper boundary was assumed to be homogeneous in surfaces parallel to the topography. The temperature was also assumed to be homogeneous in surfaces parallel to the topography, but

only at grid heights of 300 m above the terrain. (This level defines the top of the inversion in the LAX temperature profile.) Values at levels intermediate between the surface and the level aloft at which horizontal gradients were specified were obtained by linear interpolation in the vertical. Many runs were made in which these guesses were varied; these will not be described here, but suffice it to say that those that departed most from this set of specified values gave grossly unrealistic results. These values of gradients aloft are also shown in Table 5.

For one of the experiments, the model was not allowed to predict winds. Instead, wind fields were derived from the RAWIN observations at 00GMT and 12GMT, 30 September and were input to the model. Wind fields at intermediate times are obtained in the computer program by linear interpolation in time. However, in this run, the divergence derived from the observations was kept in the model program. Vertical profiles of wind are also shown in Table 6. Divergence and components of the vorticity as input to the model for this run are shown in Table 7.

The observations of CO concentration available for the construction of initial fields are even less extensive, in some ways, than the meteorological observations. There were no vertical profiles available at initial time, and no measurements made over the water area. For this variable, however, the computer program was written to allow the specification of a separate vertical profile for each horizontal grid point. It was assumed that, initially, the surface concentration at a given horizontal point was valid at all vertical levels except at the upper boundary. The initial surface concentrations at CO observing stations were obtained by averaging hourly average concentrations centered at 0530 PST and 0630 PST, 29 September as given by Roth et al. (1971, Fig. 4). These were transferred to

TABLE 7
Horizontal gradients of wind as derived from the San Nicolas-Vandenberg RAWINS and surface observations.*
00GMT/30 September

z (m)	12GMT/29 September				00GMT/30 September			
	$\frac{\partial u}{\partial x}$	$\frac{\partial u}{\partial y}$	$\frac{\partial v}{\partial x}$	$\frac{\partial v}{\partial y}$	$\frac{\partial u}{\partial x}$	$\frac{\partial u}{\partial y}$	$\frac{\partial v}{\partial x}$	$\frac{\partial v}{\partial y}$
1500	$.19094 \times 10^{-4}$	$.48867 \times 10^{-4}$	$.22654 \times 10^{-5}$	$.41780 \times 10^{-5}$	0	0	0	0
900	$.58253 \times 10^{-5}$	$.15534 \times 10^{-4}$	$.61489 \times 10^{-5}$	$.14563 \times 10^{-4}$	$-.906 \times 10^{-5}$	$-.227 \times 10^{-4}$	$.324 \times 10^{-5}$	$.583 \times 10^{-5}$
450	$.14240 \times 10^{-4}$	$.37217 \times 10^{-4}$	$.14240 \times 10^{-4}$	$-.37864 \times 10^{-4}$	$-.971 \times 10^{-5}$	$-.259 \times 10^{-4}$	$.906 \times 10^{-5}$	$-.518 \times 10^{-5}$
300	$.10356 \times 10^{-4}$	$-.38835 \times 10^{-4}$	$-.16829 \times 10^{-4}$	$-.44984 \times 10^{-4}$	$-.110 \times 10^{-4}$	$.168 \times 10^{-4}$	$.647 \times 10^{-6}$	$-.350 \times 10^{-4}$
75	$-.74434 \times 10^{-5}$	$-.35500 \times 10^{-4}$	$-.18770 \times 10^{-4}$	$-.50162 \times 10^{-4}$	$-.518 \times 10^{-5}$	$-.104 \times 10^{-4}$	$-.168 \times 10^{-4}$	0.570×10^{-5}
2	$-.87084 \times 10^{-4}$	$-.27710 \times 10^{-4}$	$.19854 \times 10^{-4}$	$-.58019 \times 10^{-4}$	$.145 \times 10^{-4}$	$-.262 \times 10^{-4}$	$-.244 \times 10^{-4}$	$.248 \times 10^{-4}$
0	0	0	0	0	0	0	0	0
-200	0	0	0	0	0	0	0	0

12GMT/30 September

z (m)	12GMT/30 September			
	$\frac{\partial u}{\partial x}$	$\frac{\partial u}{\partial y}$	$\frac{\partial v}{\partial x}$	$\frac{\partial v}{\partial y}$
1500	0	0	0	0
900	$.647 \times 10^{-5}$	$.712 \times 10^{-5}$	$-.435 \times 10^{-5}$	0.324×10^{-5}
450	$.129 \times 10^{-4}$	$.311 \times 10^{-4}$	$-.149 \times 10^{-4}$	$-.350 \times 10^{-4}$
300	$.117 \times 10^{-4}$	$.272 \times 10^{-4}$	$-.117 \times 10^{-4}$	$-.201 \times 10^{-4}$
75	$.117 \times 10^{-4}$	$.265 \times 10^{-4}$	$-.647 \times 10^{-5}$	$-.777 \times 10^{-5}$
2	$-.217 \times 10^{-4}$	$.493 \times 10^{-5}$	$-.517 \times 10^{-4}$	$-.855 \times 10^{-8}$
0	0	0	0	0
-200	0	0	0	0

* All units in sec^{-1} .

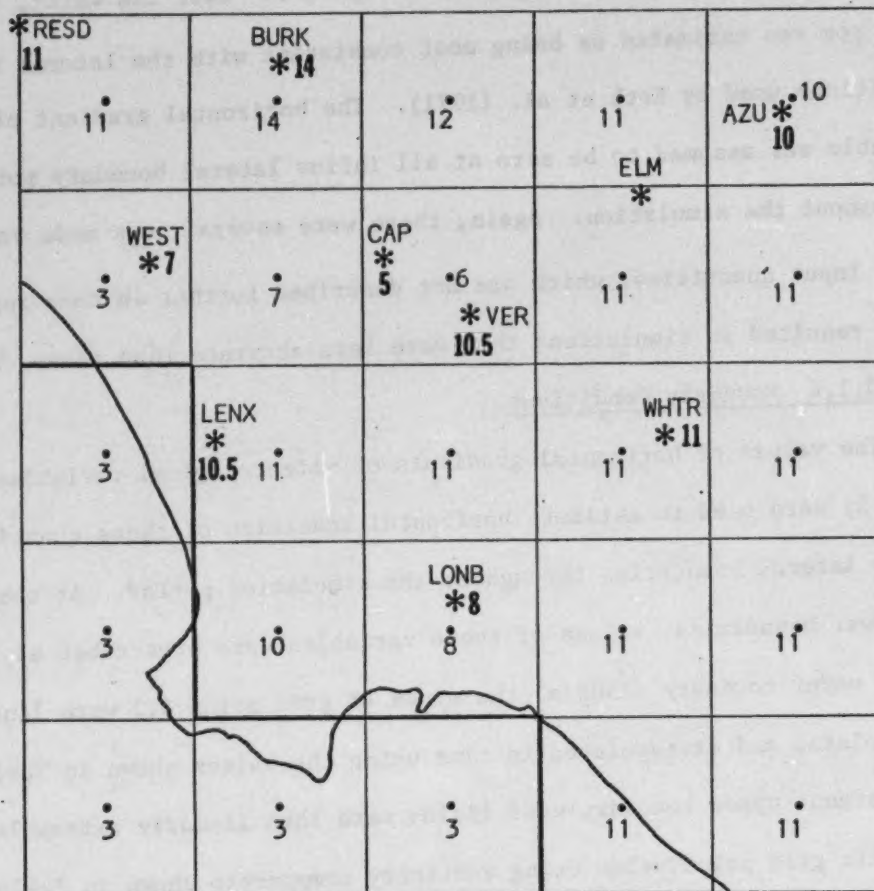
the model grid in the manner shown in Figure 7. Over the water, the value of 3 ppm was estimated as being most consistent with the lateral boundary conditions used by Roth et al. (1971). The horizontal gradient of this variable was assumed to be zero at all inflow lateral boundary points throughout the simulation. Again, there were several runs made varying these input quantities, which are not described further in this report, and which resulted in simulations that were less accurate than those shown here.

3.1.4 Boundary Conditions

The values of horizontal gradients of meteorological variables (see Table 5) were used to estimate horizontal advection of these quantities at inflow lateral boundaries throughout the simulation period. At the upper and lower boundaries, values of these variables were prescribed as follows. At the upper boundary (1500 m) the winds at grid point 3,2 were linearly interpolated and extrapolated in time using the values shown in Table 6. Nondivergent upper boundary wind fields were then linearly extrapolated from this grid point value using vorticity components shown in Table 7. All other meteorological variables are held constant in time at the values shown in Table 5 at the upper and lower boundaries.

CO concentration was input as 3 ppm at the upper boundary. The horizontal gradient was assumed to be zero at inflow lateral boundaries. At the air-land interface, the vertical flux of CO was specified as in Roth, et al. (Appendix A, and p. 22). Their fluxes, defined on the fine-grid shown in Figure 2, were averaged to the coarser grid shown in the same figure. At the air-water interface, the vertical flux of CO was assumed to be zero.

Other boundary and interface conditions required by the model are implicitly specified by the information given in Section 2.0 and Table 3.



Key	
*	Observed
•	Grid Point

Figure 7. Observed and grid point initial values of CO (ppm) over the modelled region.

3.2 The Experiments

There were a total of 40 test simulations carried out during the course of the project. With minor input changes, this is the practical equivalent of two or three simulations on the 2x2 mile mesh used in the other pollution models referred to previously. The present version of the computer program has not been designed for optimal efficiency, and the simulation of a 24-hour test period takes, in general, about 20 minutes of CPU time on the University of Connecticut shared-time 360/65 computer system. Computer costs contributed to this project by the University of Connecticut exceeded the computer budget requested from the sponsor by a significant amount.

A major problem in the preparation of this report was, therefore, the selection and presentation of interesting portions of the test output. Those runs selected for discussion in this report are listed in Table 8.

3.3 The Results

3.3.1 Results of the Base Run (Run 37)

3.3.1.1 Spatial and temporal variations of the temperature

The model simulation of the large spatial and temporal variations of temperature typical of the modelled region and period, though not completely accurate in detail, were quite encouraging. Realistic simulation of these variations is important because of the indirect influence of the temperature stratification on the evolution of pollution concentrations. It is also important as an indicator that the basic mechanisms affecting the distribution and evolution of all the dependent variables (viz., the horizontal and vertical advective transports, and the vertical mixing), in the presence of a strong surface source, are simulated with some approximation to reality.

TABLE 8

a) Test runs with $K_{\min} = 10^3 \text{ cm}^2/\text{sec}$, and variable terrain slopes.

Run Number	Meteorological Input	Properties of the Modelled Region	Interface Parameters
37 (base run)	As in Tables 4,5	Smoothed terrain slopes, both land and water contained in region.	As in Table 3
38	As in base run.	Modelled region contains level land surface and water.	As in base run.
30	As in base run	Modelled region contains doubled terrain slopes.	As in base run.

b) Test runs with $K_{\min} = 10^4 \text{ cm}^2/\text{sec}$, and other modelling variations.

Run Number	Meteorological Input	Properties of the Modelled Region	Interface Parameters
39	As in base run.	As in base run.	As in base run.
26	As in base run.	As in Run 30.	As in base run.
33	As in base run	As in Run 26, with only land.	As in base run.
31	As in base run but with observed winds input from Tables 6,7.	As in Run 26.	As in Run 26.
19	As in base run.	As in Run 26.	Land moisture parameter .2.

Figures 8 through 11 compare the regional distributions of simulated 4 m air temperatures, and observed surface temperatures at the four stations within the modelled region, and at six-hourly intervals after initial time. Figure 8 compares the distributions at noon (PST), which is the time of maximum regional variation in this set of maps. The simulated range of temporal and spatial variation of surface temperature is generally realistic, with the largest discrepancy between simulated and observed temperatures evident in the southern part of the modelled region. Grid cell 5,4, as has already been mentioned, was treated as a land grid cell. This could account for the over-prediction of surface temperatures at later times (especially at 18PST) evident in the vicinity of stations LONB and NTB. In any case, use of a finer horizontal grid mesh should be the first measure attempted in future experiments to try to improve the simulation accuracy.

Time series of observed surface temperatures at the four observing stations within the modelled region are shown in Figures 12 through 15. Also shown are time series of simulated 4 m air temperatures at the closest adjacent grid points to each station. Again, the simulated time and space variations are encouragingly realistic, with the most noticeable error evident in the overprediction of evening temperature in the vicinity of the two southernmost stations, and the delayed time of maximum simulated temperatures at LONB and LAX.

Simulated temperature distributions in the n - z plane, where n is directed along the map diagonal extending from the southwest corner to the northeast corner of the modelled region, are shown at six-hourly intervals in Figures 16 through 19. The large-scale topographic variation is also shown in these figures. The land-sea horizontal temperature contrasts of the daytime hours are seen to extend to heights of about 400 m above the

Figure 8. 12P/29 September

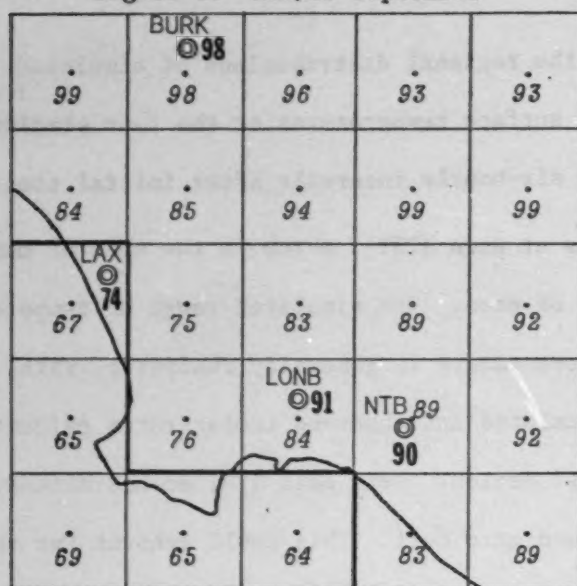


Figure 9. 18P/29 September

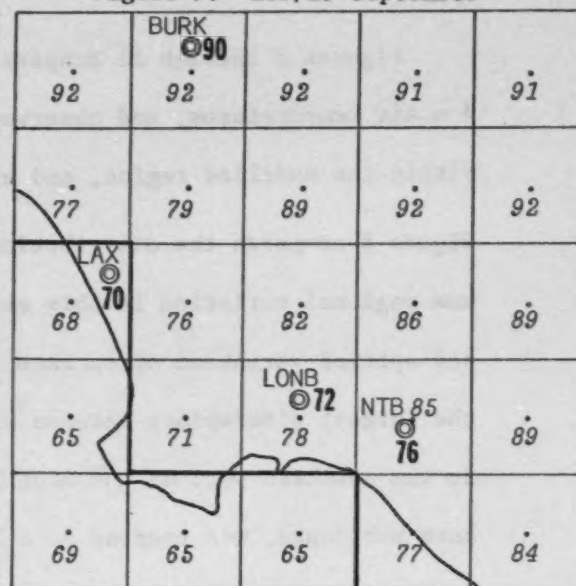


Figure 10. 00P/30 September

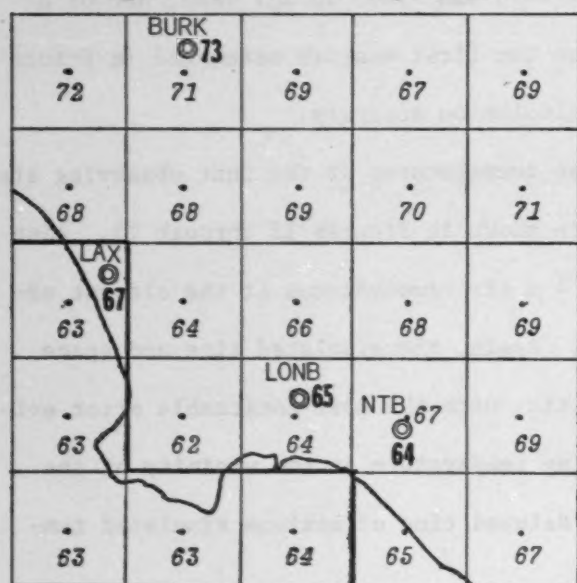
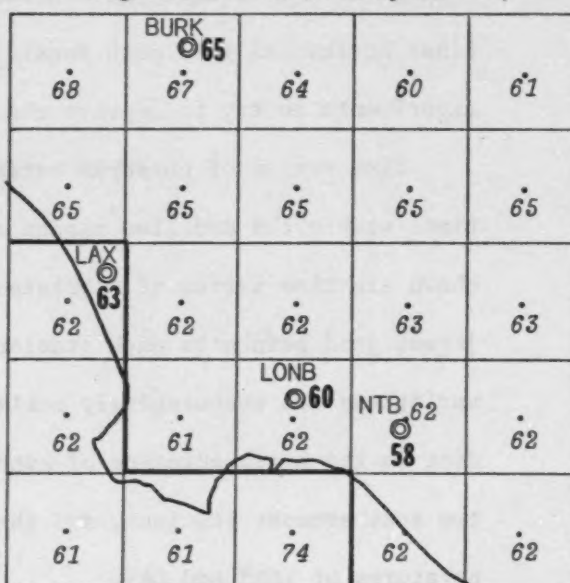


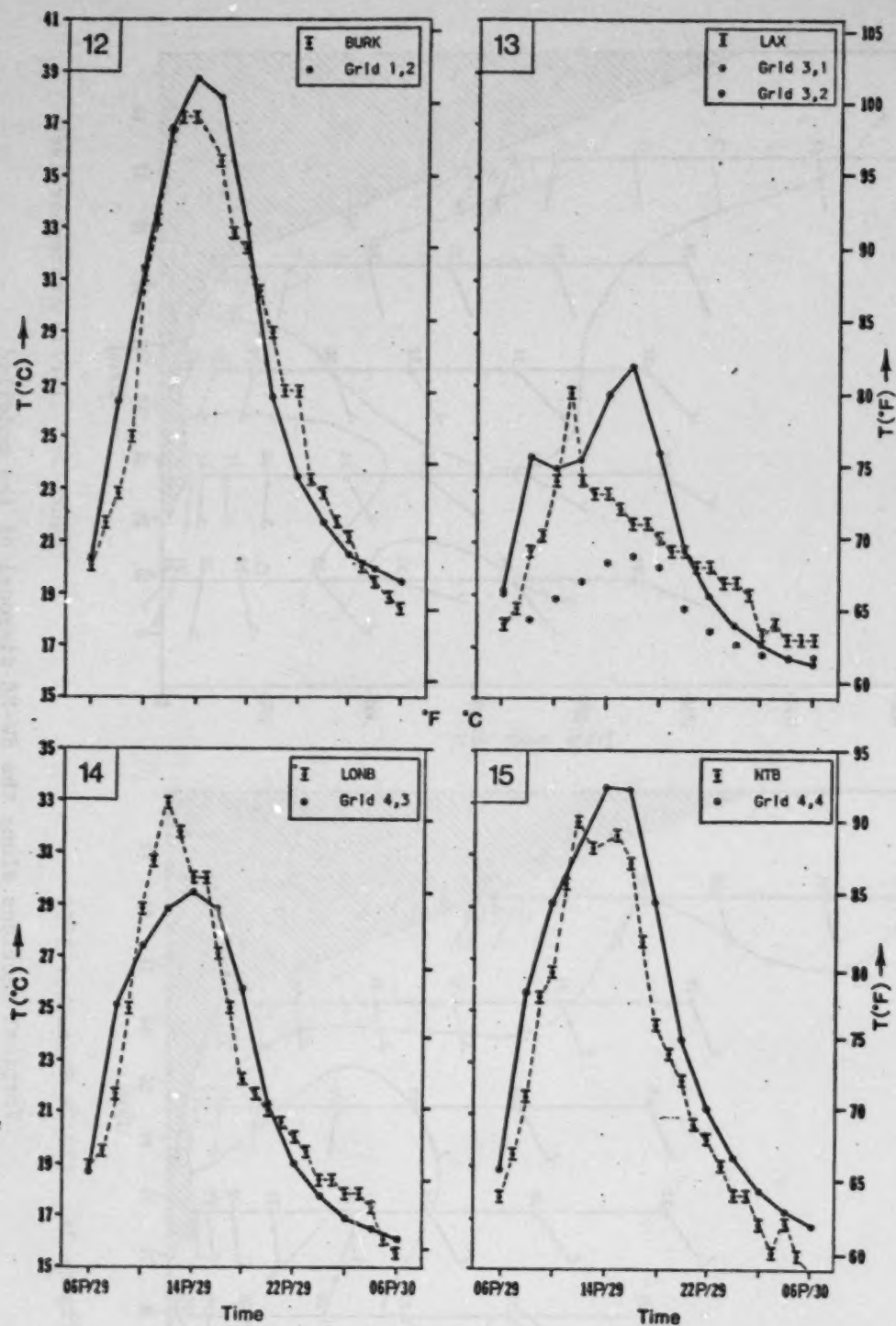
Figure 11. 06P/30 September

**Key**

● Weather Station

98 Observed temperature at station*98* Temperature predicted by base run (37)

Figures 8-11. Regional distributions of observed surface temperatures (bold face) and simulated temperatures at the four-meter grid level (italic) for the base run (un 37). Both fields are shown at six-hourly intervals.



Figures 12 - 15. Time series of observed surface temperature at the four weather stations in the modelled region; and of simulated air temperatures at the 4 m grid level and at horizontal grid points in the vicinity of the station.

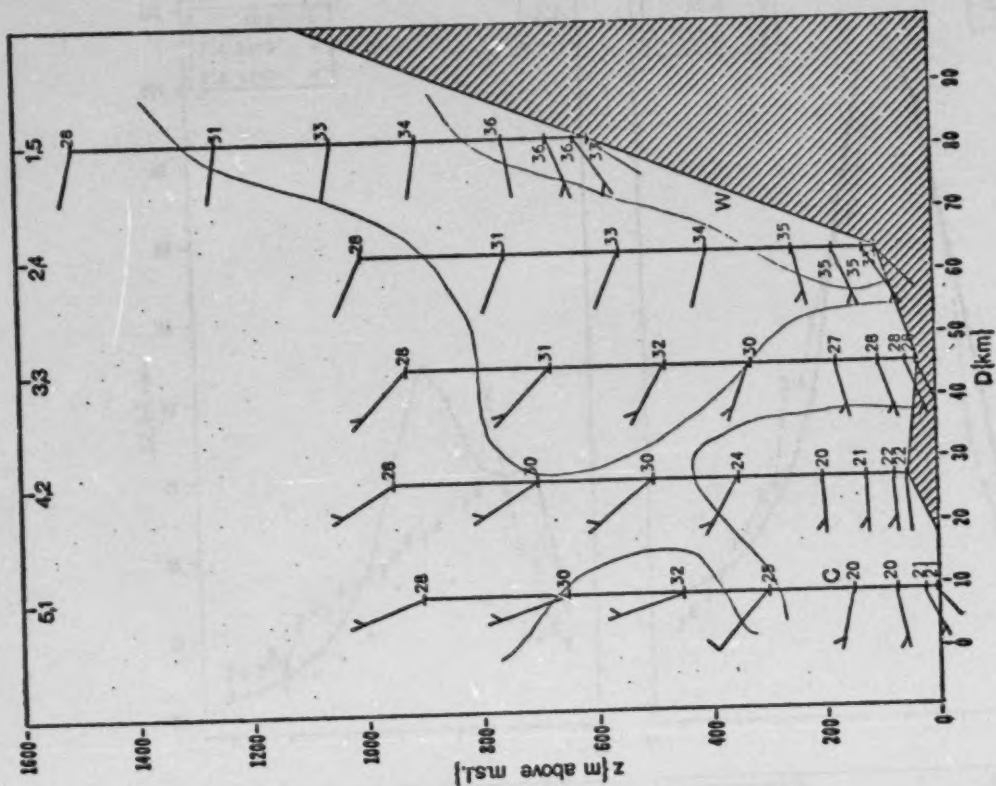


Figure 16. 12P/29 September 1969

Vertical sections along the SW-NE diagonal of the modelled region showing simulated temperatures ($^{\circ}\text{C}$) and simulated winds. Note that winds are plotted as on a conventional weather map.

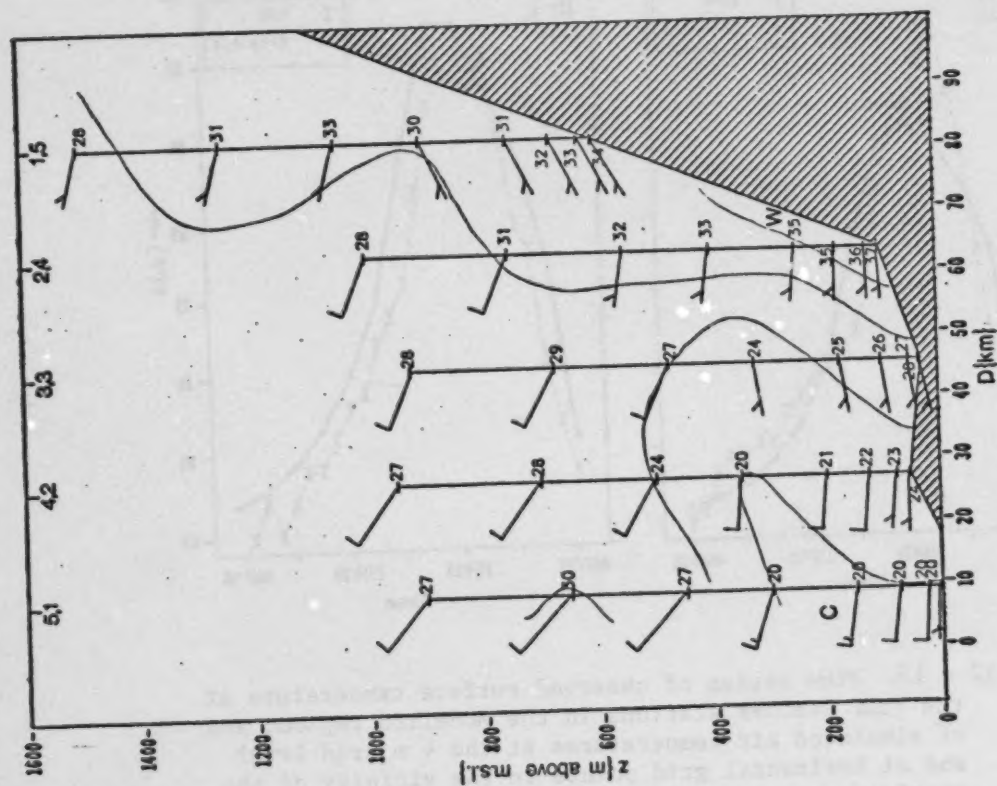


Figure 17. 18P/29 September 1969

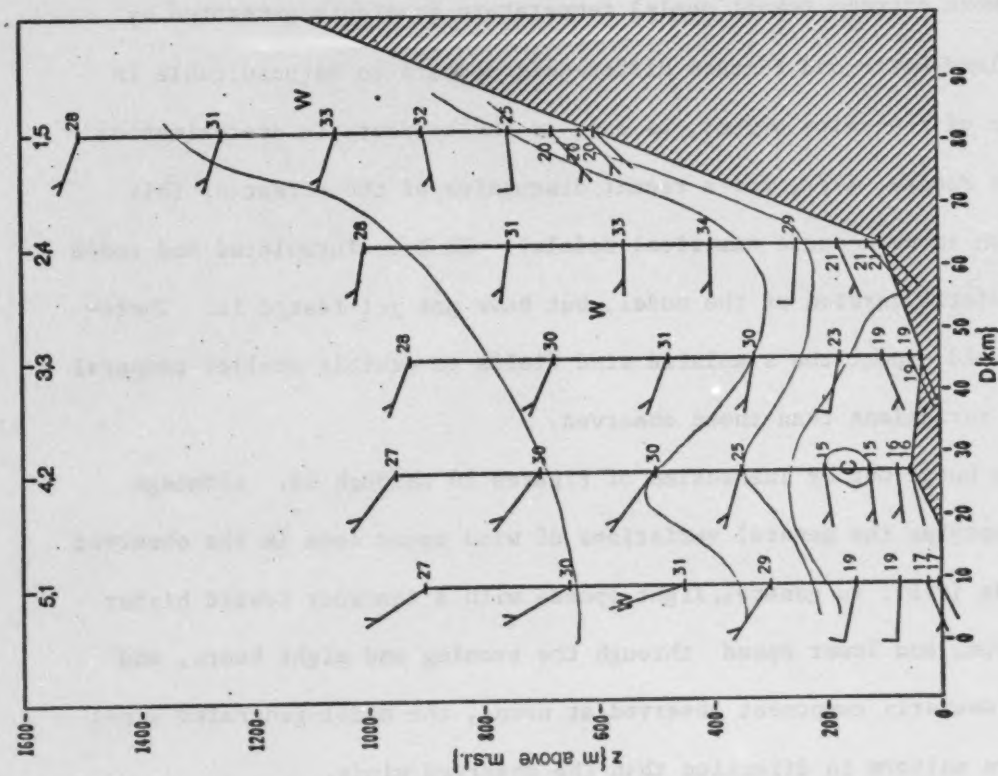


Figure 18. 00P/30 September 1969

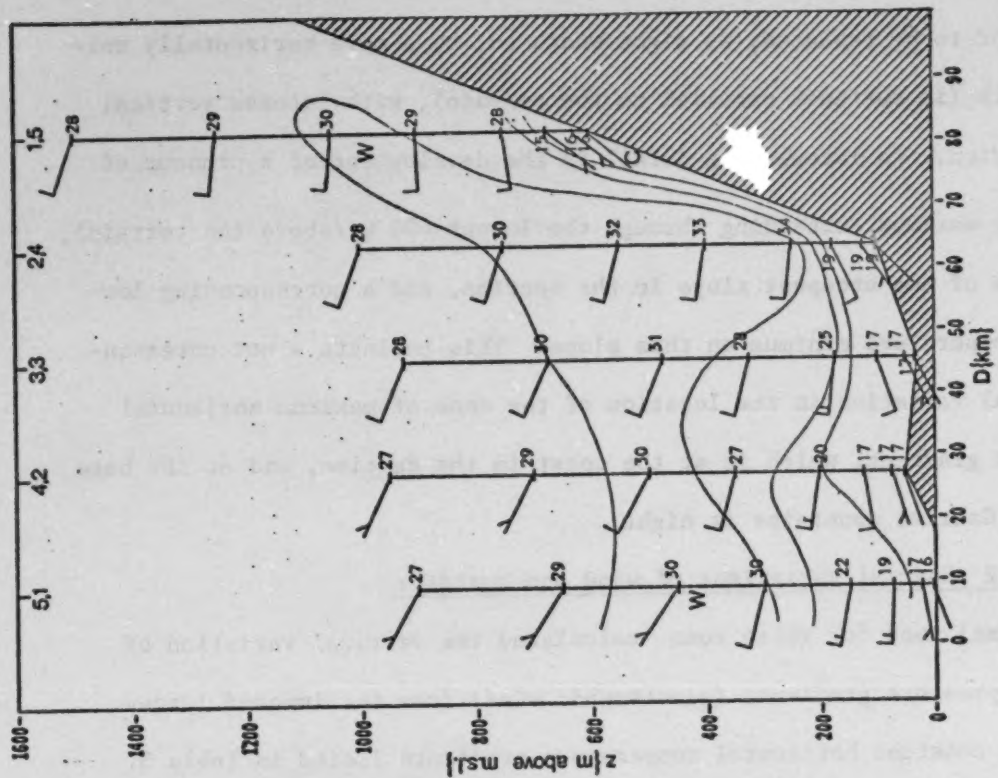


Figure 19. 06P/30 September 1969

Vertical sections along the SW-NE diagonal of the modelled region showing simulated temperatures ($^{\circ}\text{C}$) and simulated winds. Note that winds are plotted as on a conventional weather map.

terrain, and to be replaced, as night wears on, by a more horizontally uniform pattern (in surfaces parallel to the terrain), with intense vertical stratification. An interesting detail is the development of a pronounced temperature maximum, extending through the lowest 400 m (above the terrain), at the base of the steepest slope in the section, and a corresponding low-altitude temperature minimum on this slope. This reflects a not unreasonable diurnal variation in the location of the zone of maximum horizontal temperature gradient, which is at the coast in the daytime, and at the base of the San Gabriel mountains at night.

3.3.1.2 Spatial variations of wind and humidity

The model used for these runs calculated the vertical variation of horizontal pressure gradients (geostrophic wind) from the imposed large-scale, time constant horizontal temperature gradients listed in Table 5. The use of more extreme (small scale) temperature gradients generated by more local land-water and terrain differences appears to be unsuitable in this portion of the calculations, as long as the hydrostatic approximation is used (see Pielke, 1972, for a recent discussion of the effect of this approximation in meso-scale numerical models). We have formulated and coded a non-hydrostatic version of the model, but have not yet tested it. Therefore, one would expect the simulated wind fields to exhibit smaller temporal and spatial variations than those observed.

This is borne out by inspection of Figures 20 through 23. Although the model captures the general variations of wind speed seen in the observed surface winds (viz., in general, light speeds with a tendency toward higher speed at noon, and lower speed through the evening and night hours, and the general westerly component observed at noon), the model-generated winds are much more uniform in direction than the observed winds.

Figure 20. 12P/29 September

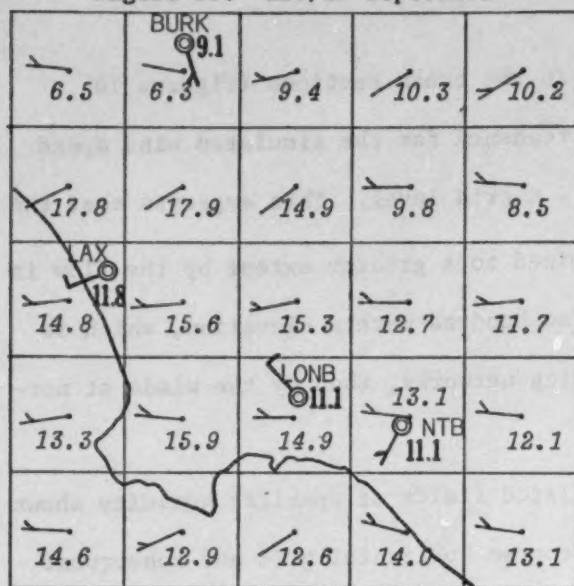


Figure 21. 18P/29 September

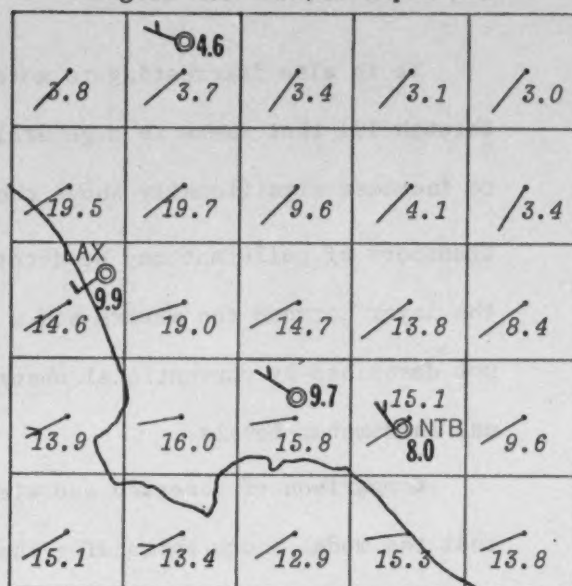


Figure 22. 00P/30 September

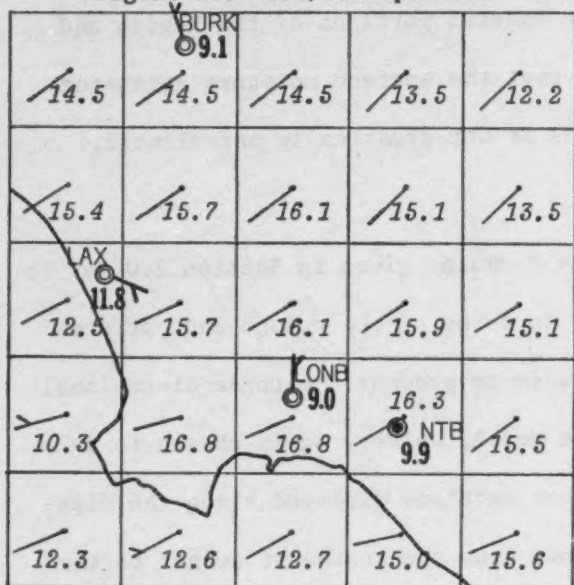
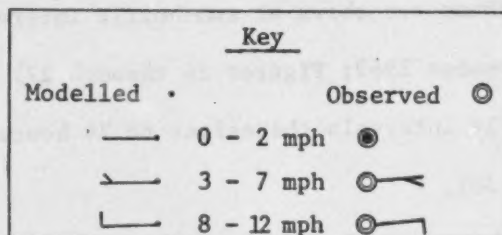
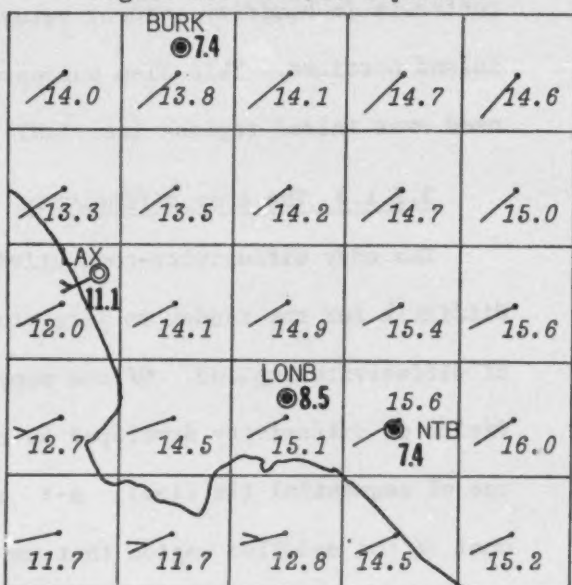


Figure 23. 06P/30 September



Figures 20 - 23. Maps of observed surface winds and specific humidity (g/kg), and of simulated wind and humidity at the 4m grid level, at six-hourly intervals. Observed humidity values are in bold face, and the simulated humidity values are in italic.

It is also interesting to note in the cross sections (Figures 16 through 19) that there is a general tendency for the simulated wind speed to increase significantly above the 4 m grid level. This suggests that the transport of pollutant may be determined to a greater extent by the flow in the layer between ten meters and a few hundred meters elevation, which is not described by conventional observing networks, than by the winds at normal anemometer levels.

Comparison of observed and simulated fields of specific humidity shows that the model (notwithstanding the coarse horizontal grid and subsequent smoothing of terrain features) is able to generally simulate the large contrasts in humidity evident between coastal portions of the region and inland portions. This also suggests that the surface moisture parameter used over inland regions (see Table 3) is not drastically unrealistic.

3.3.1.3 The eddy diffusivity

The eddy diffusivity-conductivity formulas given in Section 2.0 may be difficult for the reader to interpret in terms of the values and patterns of diffusivity implied. Of the many ways to present the three-dimensional fields of diffusivity developed by the model, we have again chosen to make use of sequential (in time), n-z cross sections directed along the diagonal of the modelled region that extends from the southwest corner to the northeast corner. These are shown at two-hourly intervals from initial time (06PST, 29 September 1969; Figures 24 through 27) to noon of the same day; and at six-hourly intervals thereafter to 24 hours after initial time (Figures 28 through 30).

The somewhat arbitrary value for the minimum free atmospheric value imposed, viz. $10^3 \text{ cm}^2/\text{sec}$, dominates throughout most of the vertical slice shown, at most of these times. One of the experiments to be described later

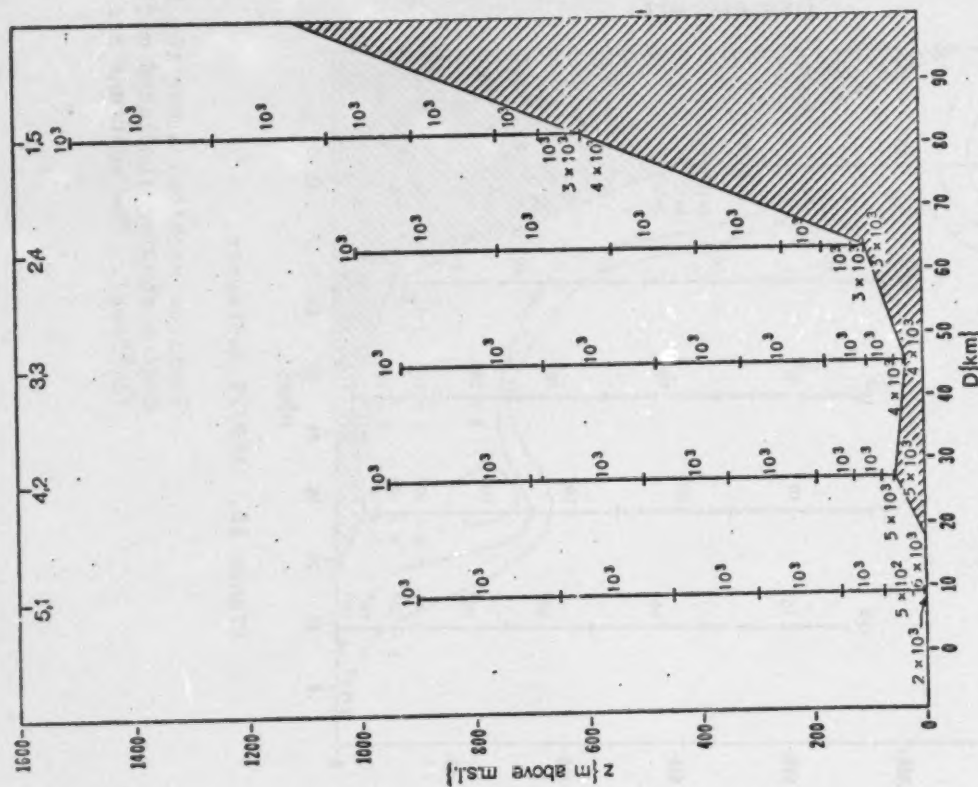
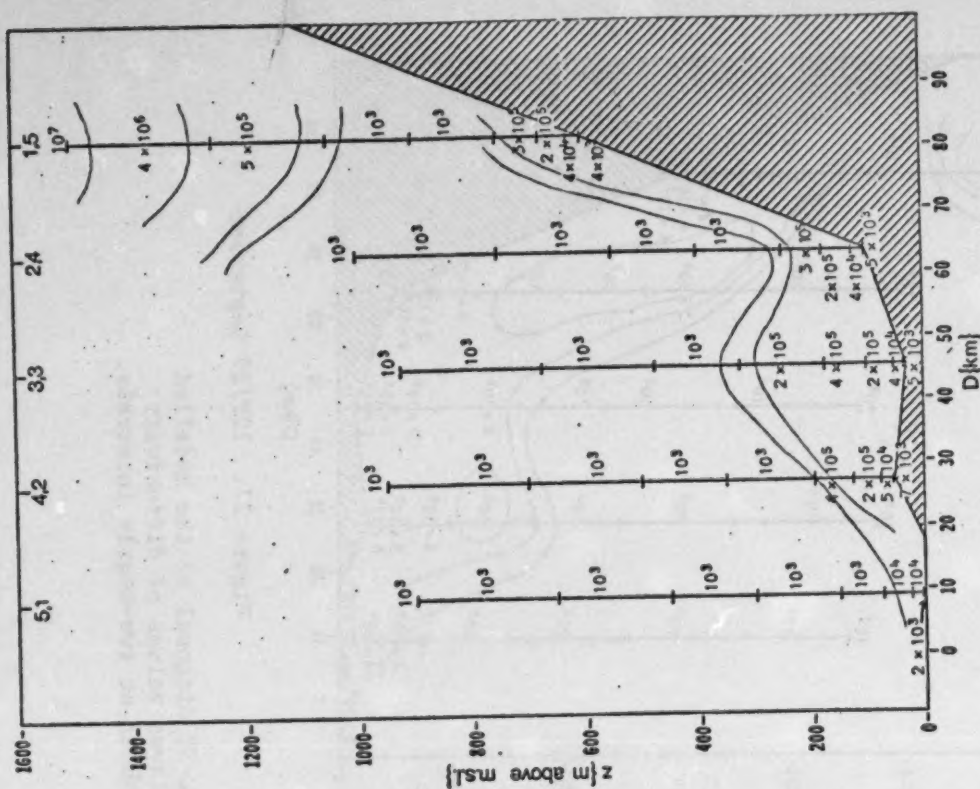


Figure 25. 08P/29 September

Figure 24. 06P/29 September

Vertical sections along the SW-NE diagonal of the modelled region showing simulated mid-layer values of diffusivity (cm^2/sec). The sections are shown at two-hourly intervals.

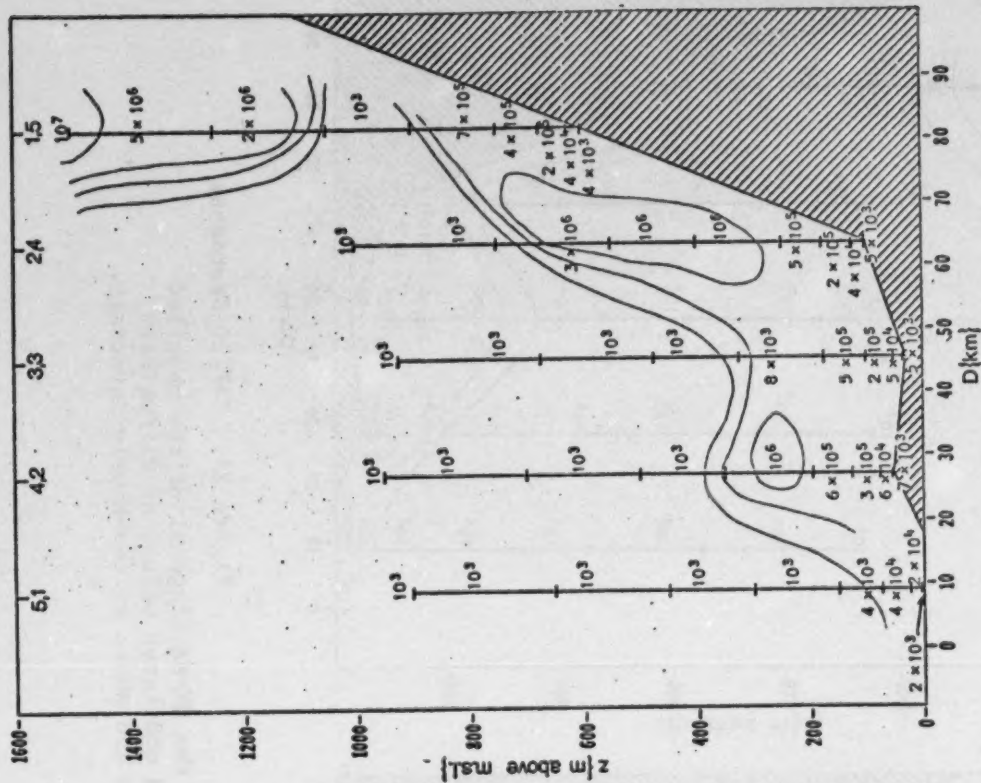


Figure 26. 10P/29 September

Vertical sections along the SW-NE diagonal of the modelled region showing simulated mid-layer values of diffusivity (cm^2/sec). The sections are shown at two-hourly intervals.

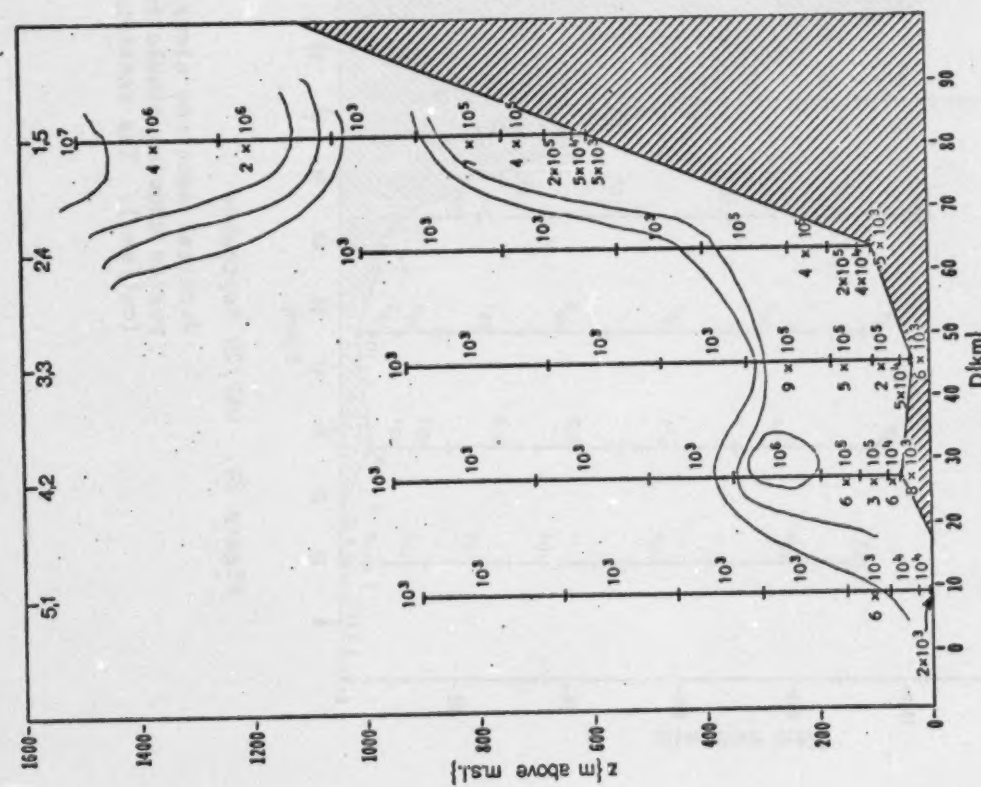


Figure 27. 12P/29 September

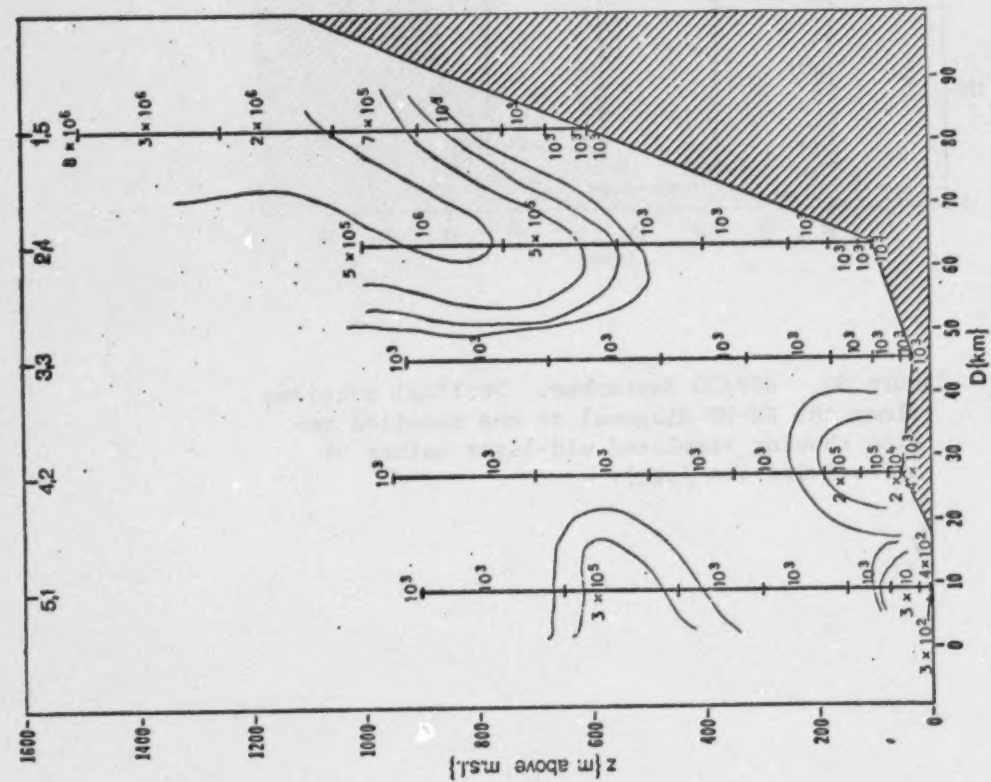


Figure 28. 18P/29 September

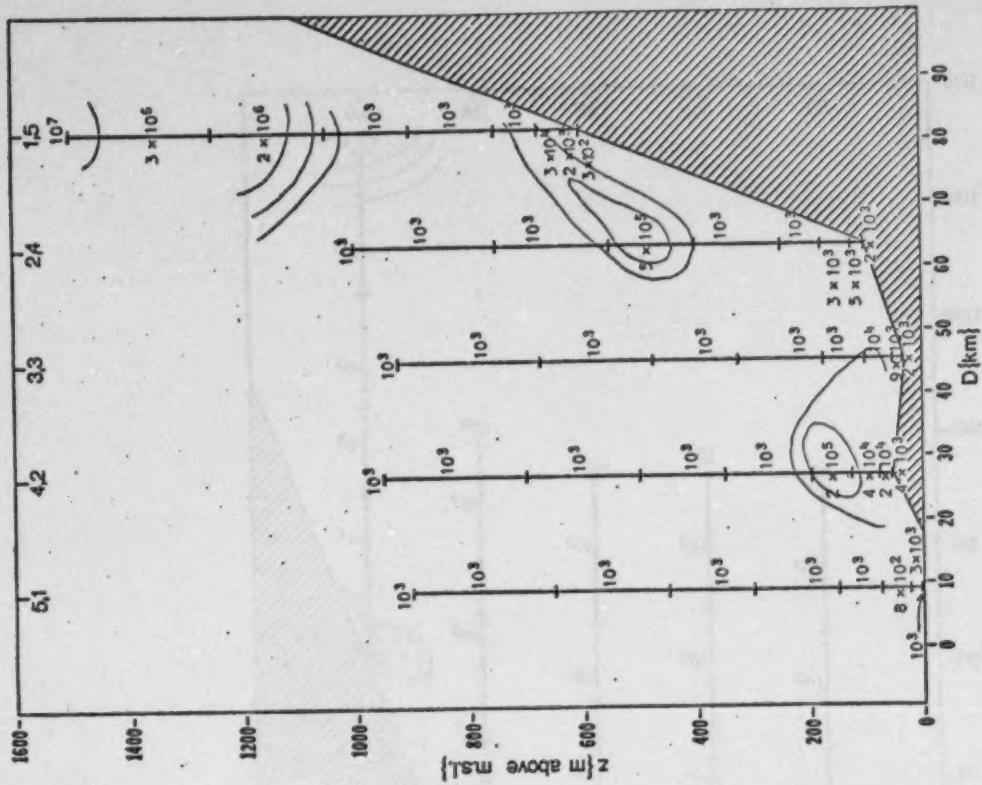
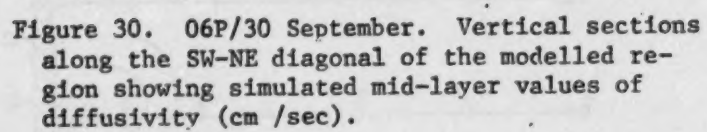


Figure 29. 00P/30 September

Vertical sections along the SW-NE diagonal of the modelled region showing simulated mid-layer values of diffusivity (cm^2/sec). The sections are shown at six-hourly intervals.



shows that the accuracy of those simulated ground-layer concentrations, for which validation data are available, is not very sensitive to an order of magnitude increase in this value. Otherwise the simulated behavior of this parameter, while not verifiable in detail, and (presumably) not accurate in detail, is not unreasonable in general.

The major expected features are the development during the morning hours of a layer of more intense mixing below the inversion base over land which extends by noon to a height of 300 to 400 m above the surface; its disappearance by late afternoon, and throughout the nighttime hours; and its absence over water. A questionable detail is the development of an elevated layer (based at 600 m and above) of intense mixing, separated from the surface layer by an intermediate minimum of less intense diffusion over the northeastern part of the cross section. It may be determined in the future that this is not a realistic feature. For the present, as will be seen in Sections 3.3.1.5 and 3.3.3.2, there is some indirect evidence in the accuracy of simulated pollutant variations at AZU and BURK, that this is a realistic feature of the simulated meteorology.

3.3.1.4 The vertical velocity

The simulated vertical velocity, like the simulated diffusivity, cannot be directly compared to observations. Thus, we can only infer the validity of the simulated patterns from the accuracy of simulation of other variables, which are sensitive to errors in the vertical velocity to an undetermined extent.

The formulation used in this model (see Section 2.0) separates the calculated vertical velocity into two terms, one evaluated from the divergence of the horizontal wind in terrain parallel surfaces; and one evaluated from the scalar product of the local horizontal wind and the terrain

slope. One would expect the simulated vertical velocity, therefore, to reflect the terrain scales defined by the horizontal grid; and to contain more spatial variability when finer grids are used. Confirmation of this expectation must await future experiments. Nonetheless, some readers may be interested in the general characteristics of the simulated vertical velocity fields in the coarse grid used in these experiments and we will briefly describe them here.

The divergence-induced component of the vertical velocity is shown in the previously described cross section, at six-hourly intervals, beginning at noon PST, in Figures 31 through 34. A general low-level pattern of subsidence over the water, upward motion on the coast, subsidence at the foot of the large slopes inland, and a more variable cellular structure on the steeper slopes is evident. Vertical velocity contributions from this term are of the order of one centimeter per second at a few hundred meter elevation, and appear to be more intense in the daytime.

The terrain-induced component of the vertical velocity, when added to the patterns above, produced total vertical velocities which vary spatially in the same general manner, but which exhibit much less temporal variability. Two of these fields are shown in Figures 35 and 36, at noon PST on 29 September, and 06 PST on the 30th. This component, as would be expected, has no influence over the water, has at least equal influence over the coastal plain, and is definitely dominant over the steep slopes, producing total vertical velocities of order 10 cm/sec in the northeastern portion of the cross section.

The effects of the vertical velocity on the simulated thermal structure, and hence on the simulated diffusivity and subsequently the carbon monoxide concentrations, should therefore be most pronounced in this part

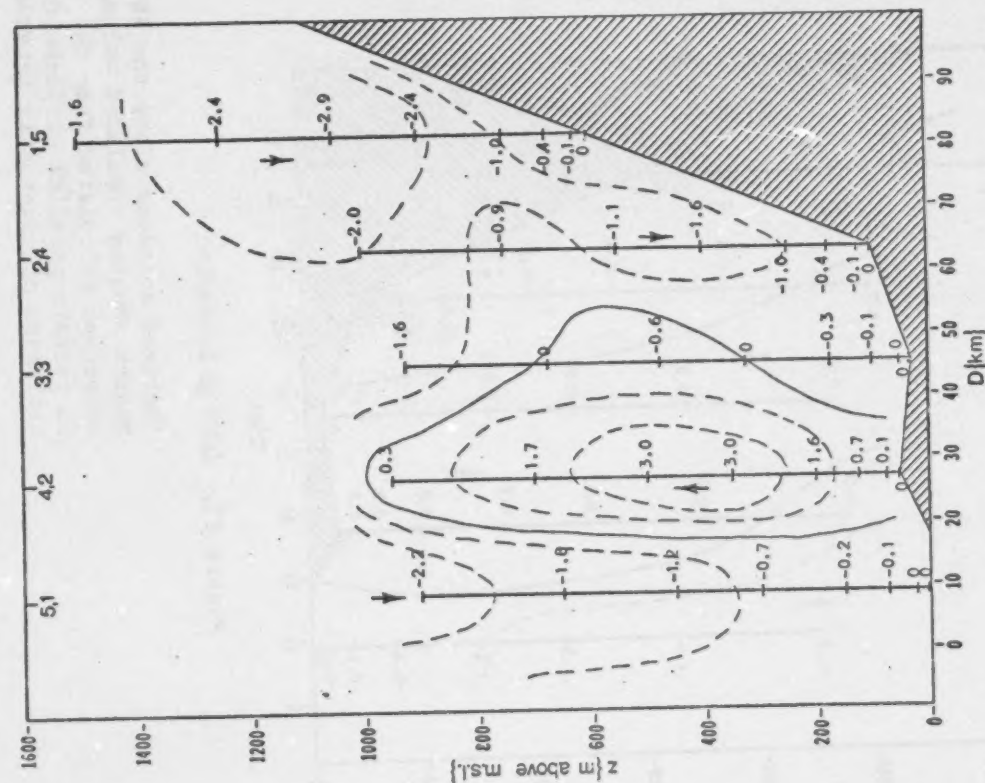


Figure 31. 12P/29 September

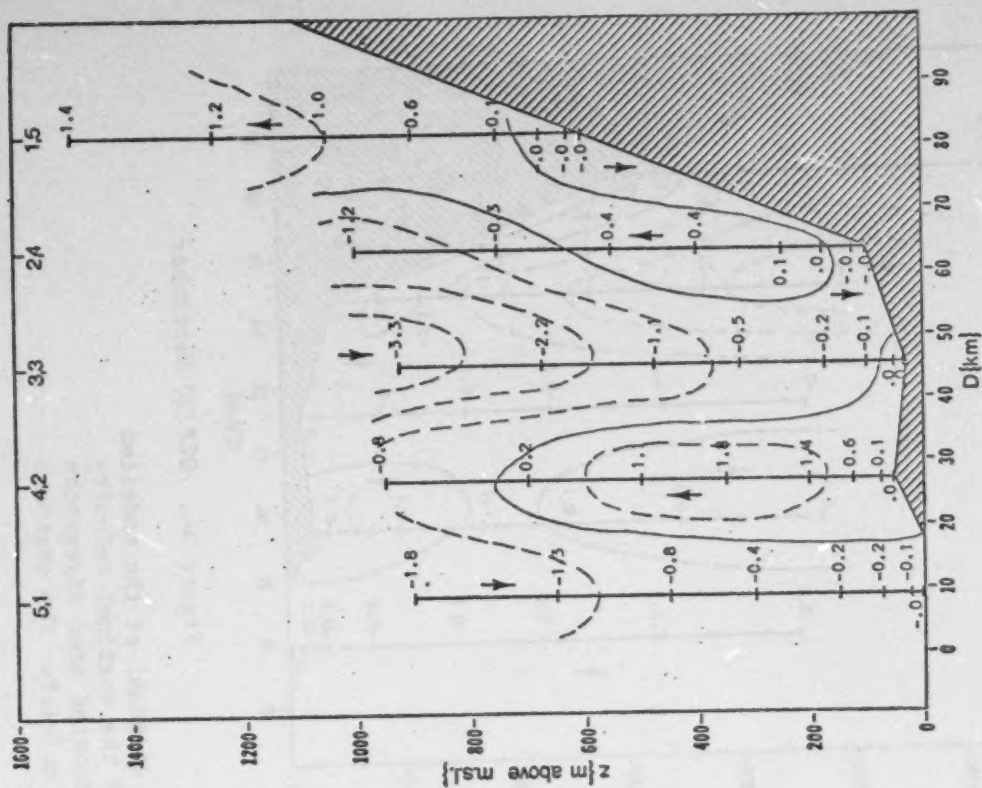


Figure 32. 18P/29 September

Vertical sections along the SW-NE diagonal of the modelled region showing simulated values of the vertical velocity component calculated from the horizontal wind divergence in terrain-parallel surfaces (w_p , cm/sec). The sections are shown at six-hourly intervals.

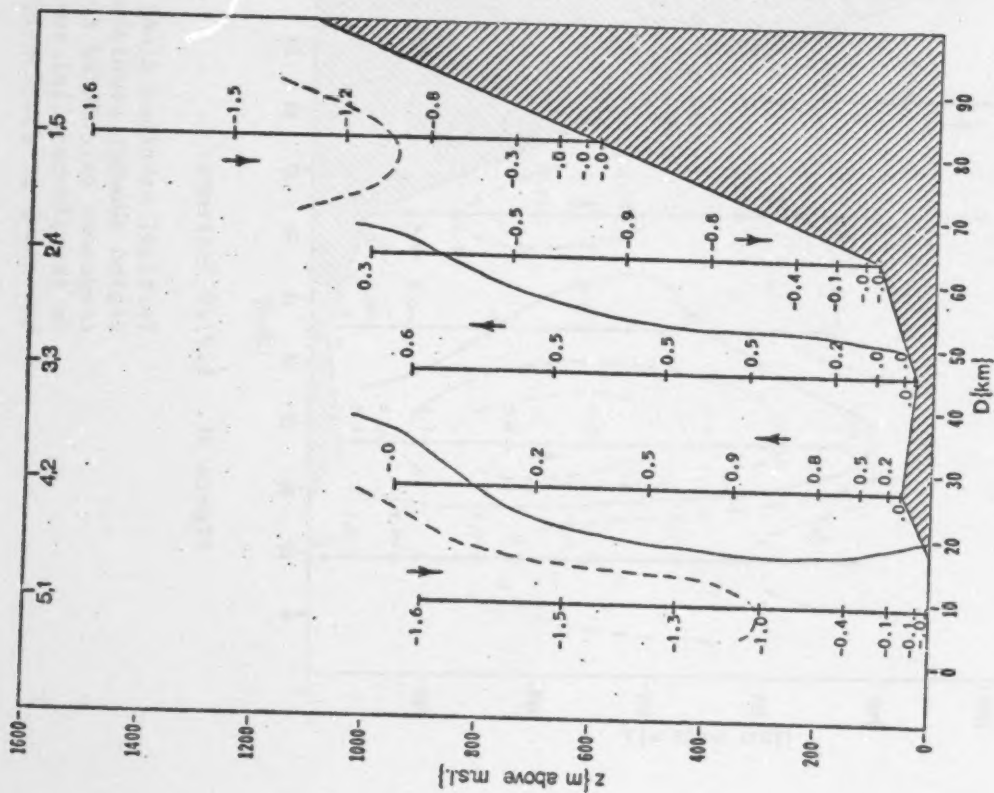


Figure 33. 00P/30 September

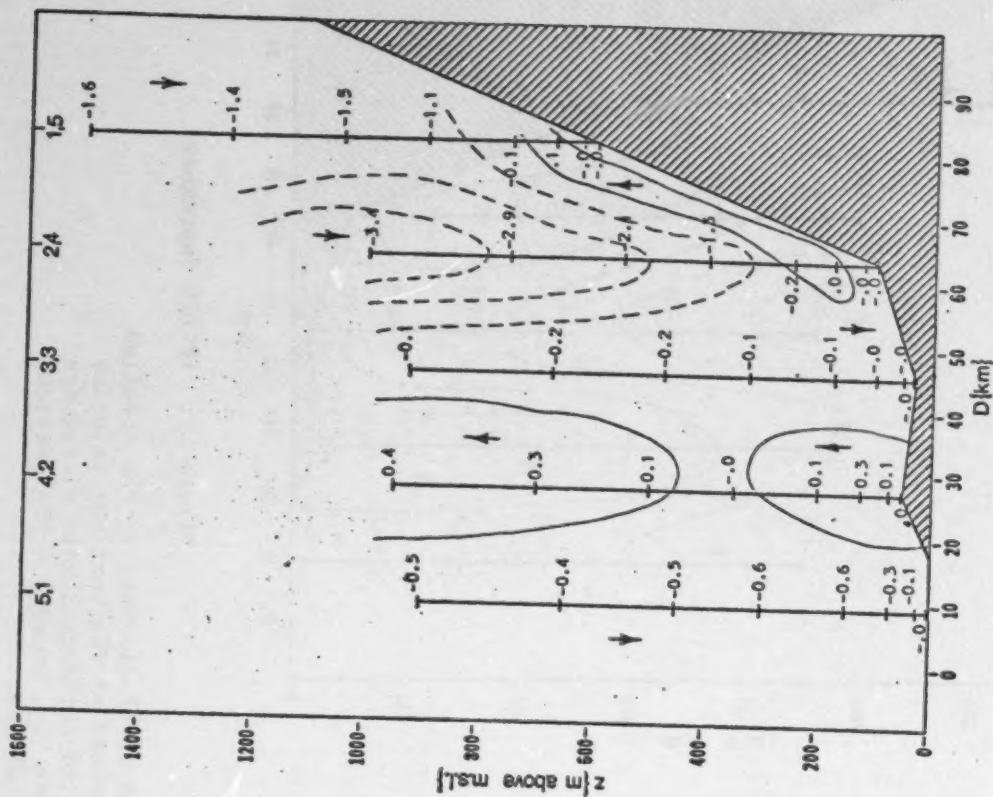


Figure 34. 06P/30 September

Vertical sections along the SW-NE diagonal of the modelled region showing simulated values of the vertical velocity component calculated from the horizontal wind divergence in terrain-parallel surfaces (w_d , cm/sec). The sections are shown at six-hourly intervals.

of the modelled region. It has already been pointed out that the detailed validity of the simulated diffusivity and vertical velocity fields must remain open to question until further validation has been carried out. It is reassuring, however, that those portions of the grid which contain the most intense and most complicated fields of these variables (i.e., the northeastern portions) are also the portions in which the most accurate simulations of ground-level concentrations of CO were produced. This will be shown in the following section.

3.3.1.5 The pollutant concentrations

The CO concentration is the key variable simulated by the model. Its spatial and temporal variations should be simulated with sufficient accuracy to justify further development of the model in this application, and/or the use of the temperature, wind, and diffusivity fields produced by this model as input to other, more complex, models of pollutant transport, diffusion, and chemistry (e.g., that of Eschenroeder and Martinez, 1971).

Maps showing observed ground-layer concentrations and simulated concentrations at the 4 m grid level, and at 2 hourly intervals from 08PST to 16PST, are shown as Figures 37 through 41 inclusive. Most discouraging are the large underestimates of CO concentration in the coastal and downtown districts at 08 and 10PST, the period of morning peak concentrations. Most encouraging are the realistic simulations at Burbank, Azusa, and El Monte throughout most of the period, in the region of most rugged topography, and the region farthest from the upwind lateral boundaries of the model. Also one might be encouraged by the fairly accurately simulated spatial variations subsequent to 10PST, when it is remembered that these were obtained with a relatively coarse horizontal grid.

The results are also presented as time series of observed CO concentra-

Figure 37. 08P/29 September

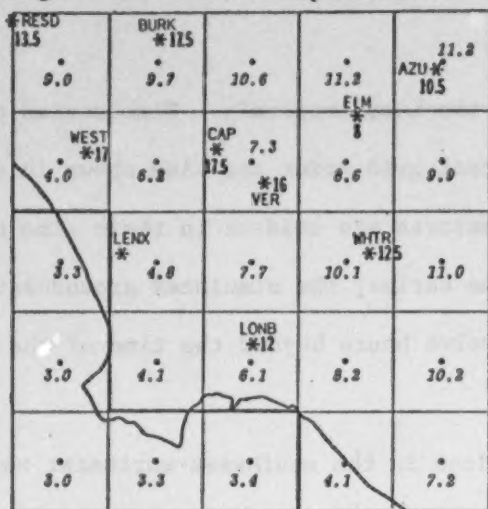


Figure 38. 10P/29 September

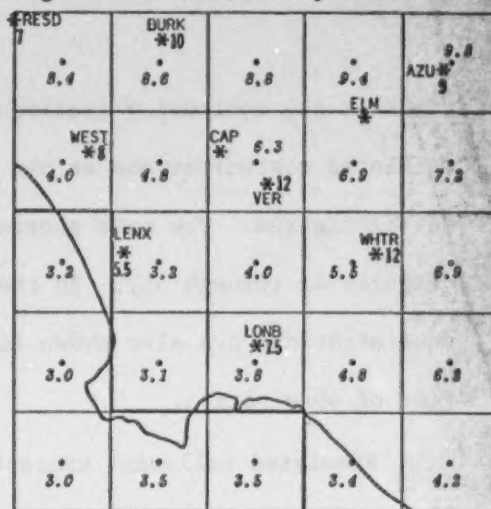


Figure 39. 12P/29 September

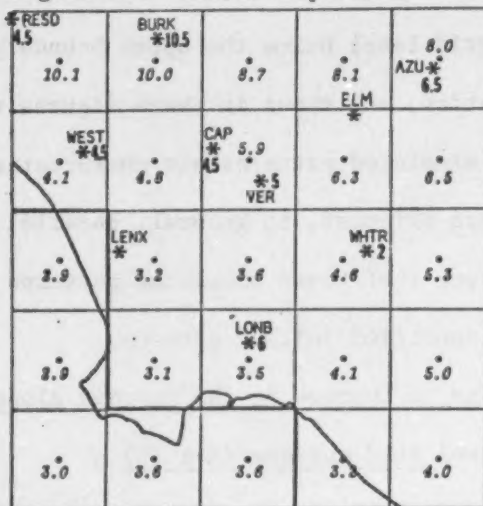


Figure 40. 14P/29 September

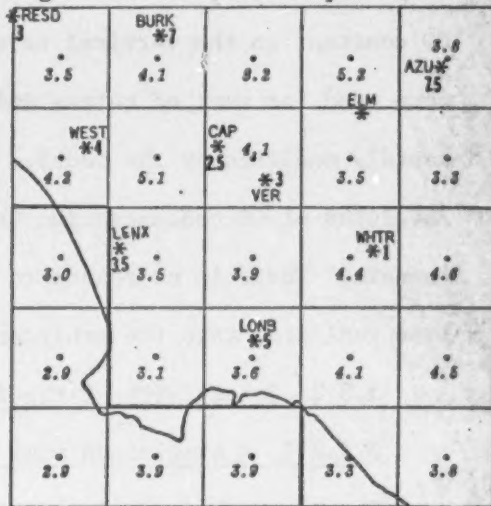
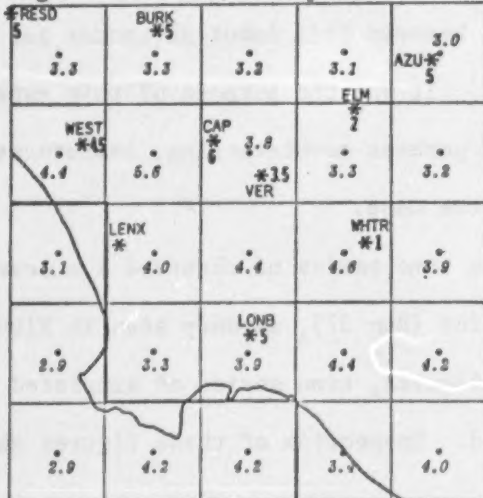


Figure 41. 16P/29 September

**Key**

- * CO Monitoring Station
- 9.8 Observed CO Concentrations at Station
- 9.8 CO Concentrations Predicted by Base Run 37

Figures 37 - 41. Maps of observed surface layer CO concentration (ppm) and simulated concentrations at the 4m grid level. Mpas are shown at two-hourly intervals.

tions at ten monitoring stations at two-hour intervals. Time series of simulated concentrations at the nearest grid point are also shown in this set of figures. The same general features are evident in these time series (Figures 42 through 51). In the time series, the simulated ground-level CO concentrations are also shown for twelve hours beyond the time of the last time of observation.

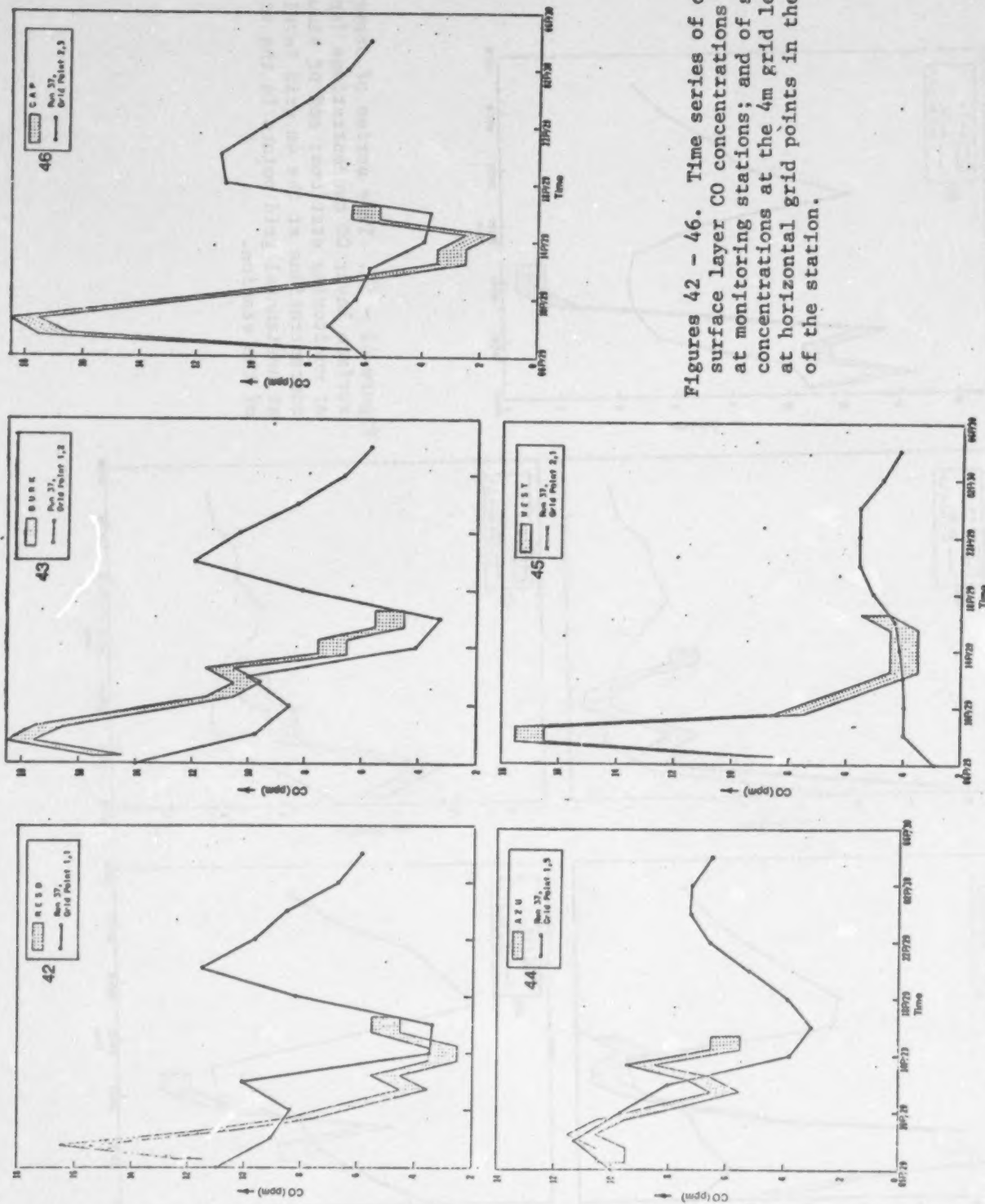
Simulated pollutant concentrations in the southwest-northeast vertical slice used previously, and at six hourly intervals, are shown in Figures 52 through 56 inclusive. The unrealistic initial vertical distributions (viz., CO constant in the vertical to one grid level below the upper boundary), that were used for want of better information, are shown in these figures to be rapidly modified by the model. The simulated patterns are characterized by isopleths of CO concentration that are oriented, in general, parallel to the terrain. There is no reason to believe that these simulated patterns are less realistic than the arbitrarily specified initial pattern.

3.3.2 Sensitivity of the Results to Changes in the Terrain Slope

3.3.2.1 A simulation with a level land surface (Run 38)

There are two experiments listed in Table 8 in which the input terrain slopes were varied. Even a cursory analysis of the modelling equations shows several direct and indirect linkages between this input parameter and the simulated ground-level CO concentrations. It was the purpose of this experiment to illustrate how these complex, and perhaps counteracting, influences affect the pollutant concentration in this one case.

Figures 57 through 66 repeat the time series of observed 4 m level CO concentrations, and the base simulation (Run 37), already seen in Figures 42 through 51. However, in the new figures, time series of simulated CO concentrations for Run 38 are also added. Inspection of these figures shows,



Figures 42 - 46. Time series of observed surface layer CO concentrations (ppm) at monitoring stations; and of simulated concentrations at the 4m grid level and at horizontal grid points in the vicinity of the station.

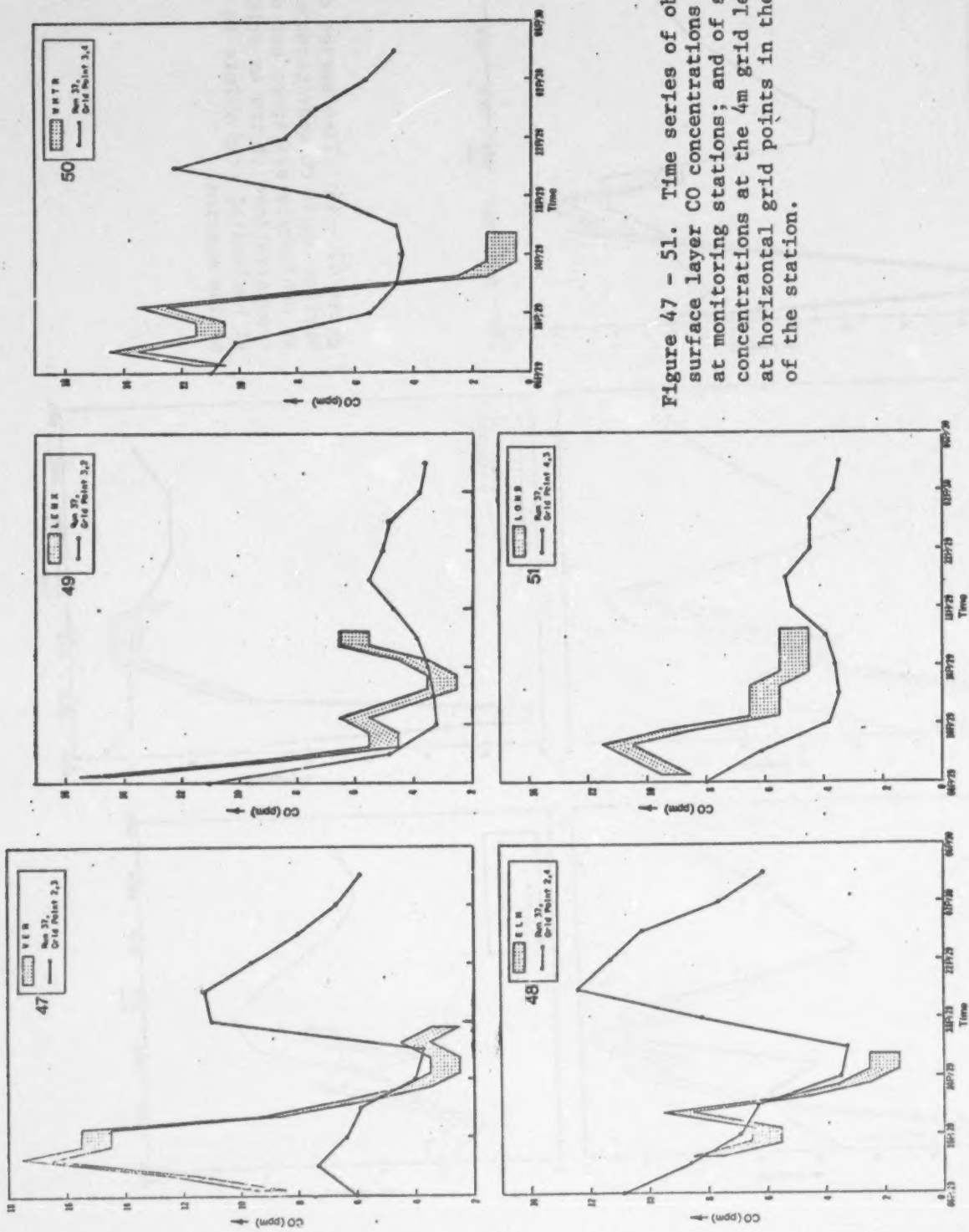


Figure 47 - 51. Time series of observed surface layer CO concentrations (ppm) at monitoring stations; and of simulated concentrations at the 4m grid level and at horizontal grid points in the vicinity of the station.

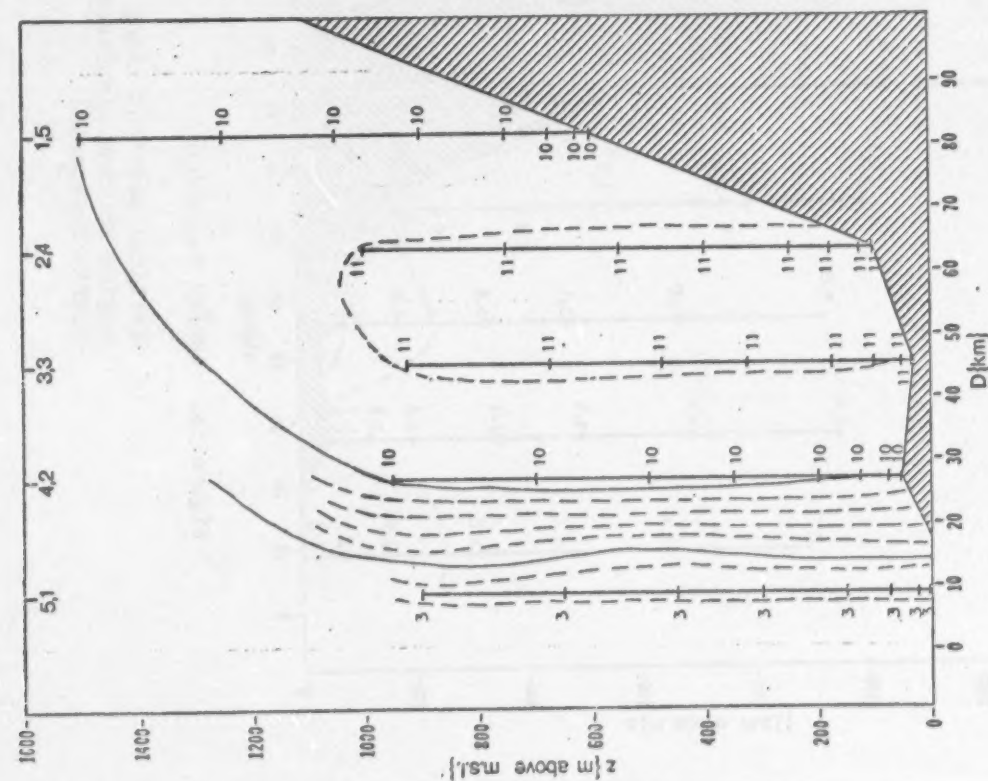


Figure 52. 06P/29 September

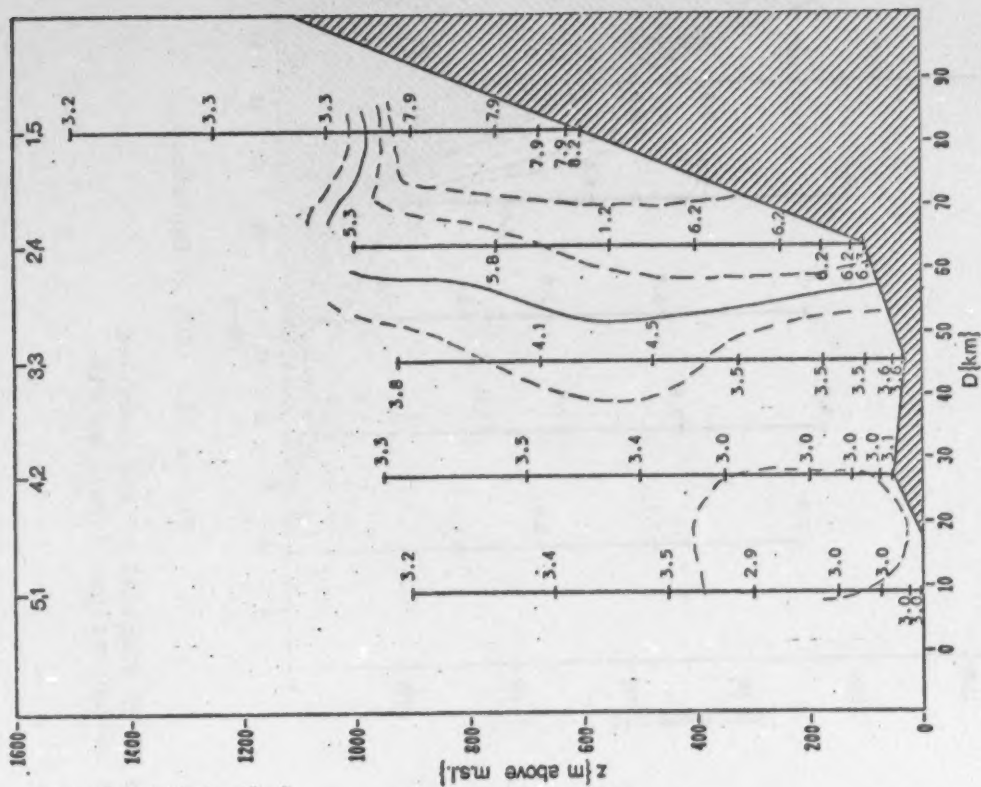


Figure 53. 12P/29 September

Vertical sections along the SW-NE diagonal of the modelled region showing simulated CO concentrations (ppm), at six-hourly intervals.

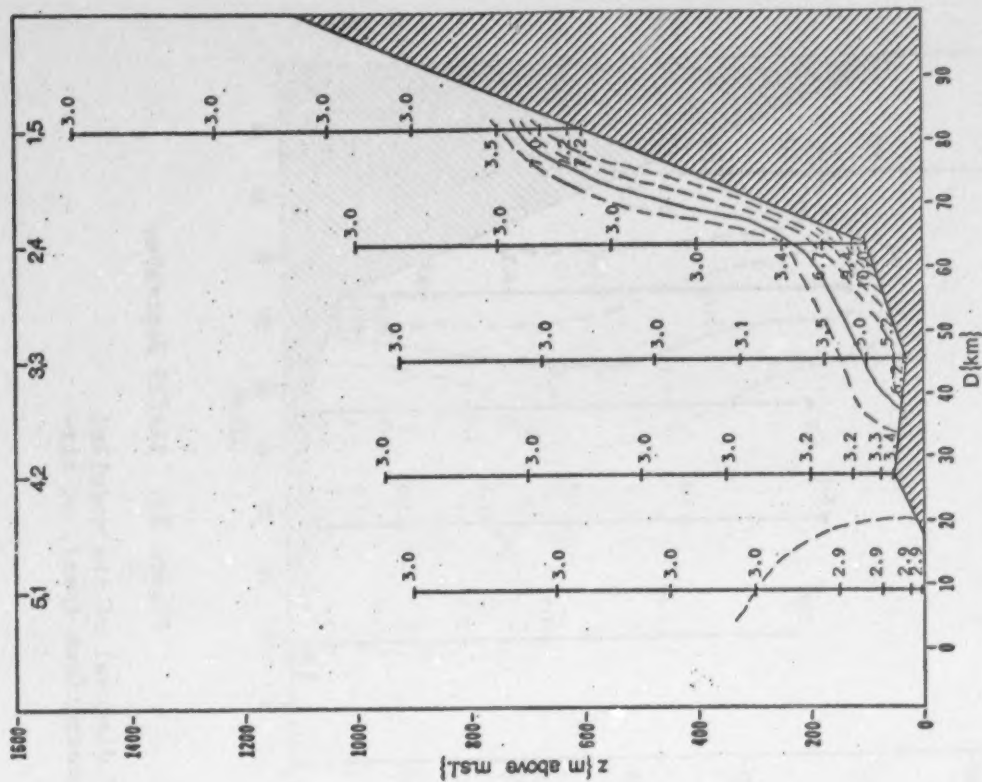


Figure 54. 18P/29 September

Vertical sections along the SW-NE diagonal of the modelled region showing simulated CO concentrations (ppm), at six-hourly intervals.

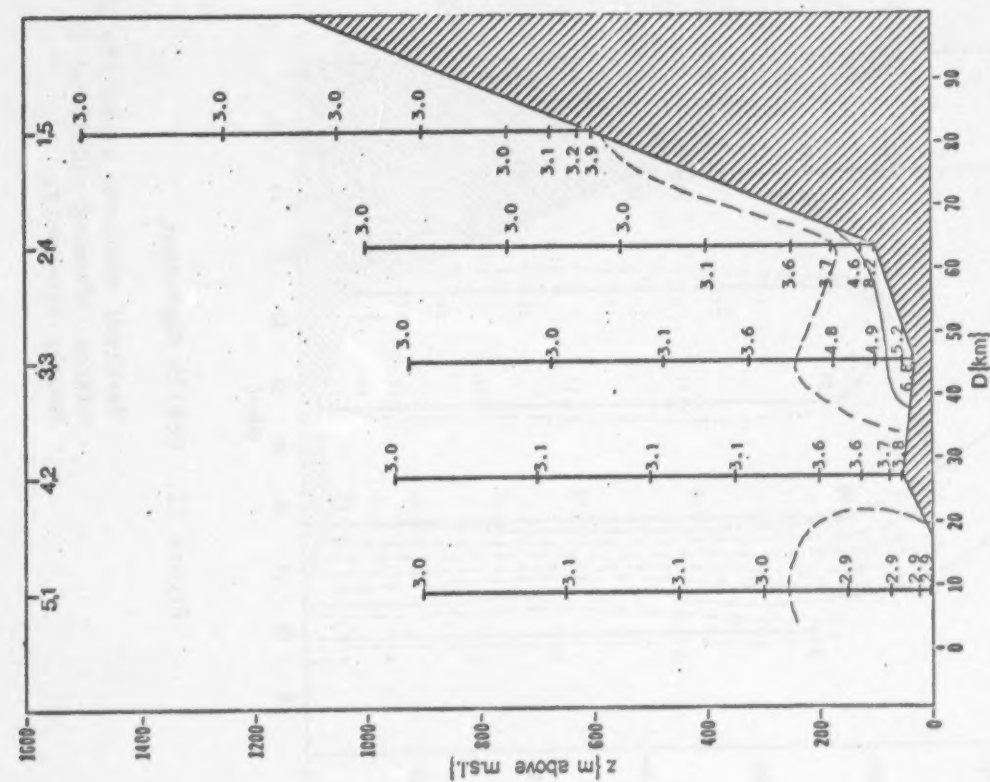


Figure 55. 00P/30 September

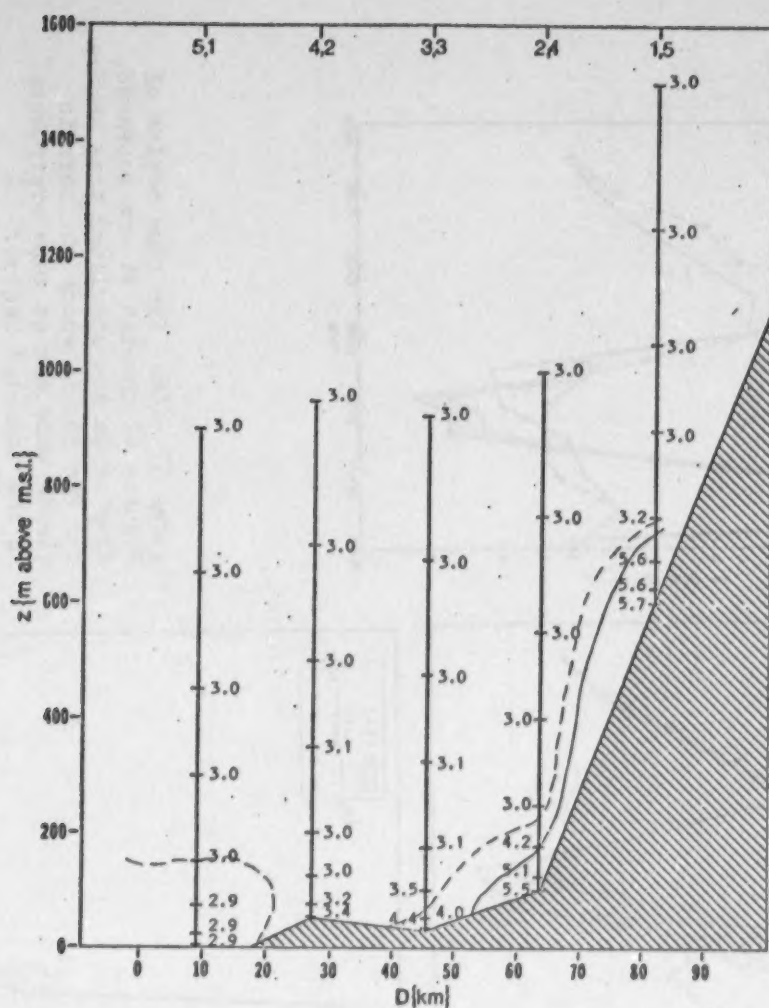
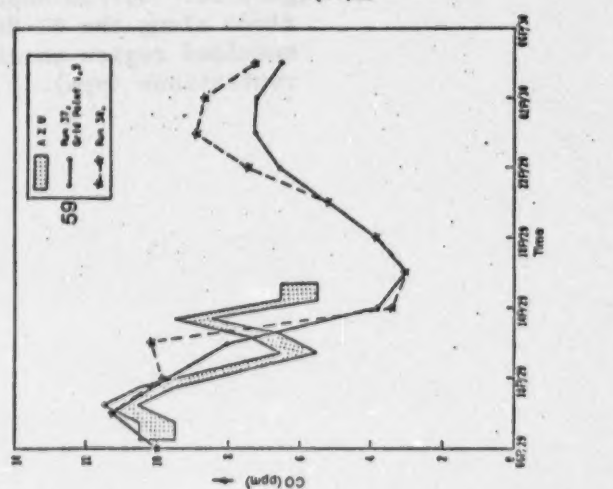
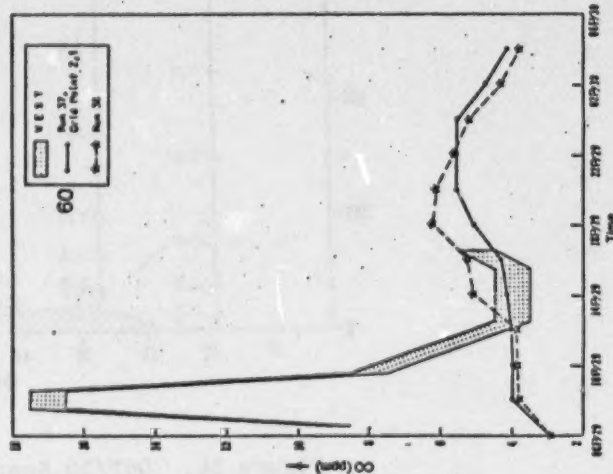
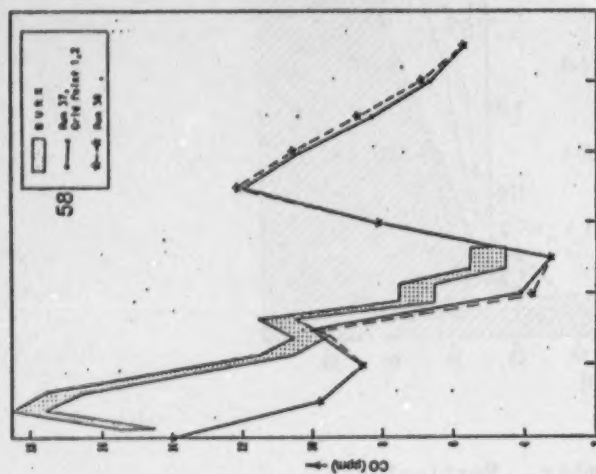
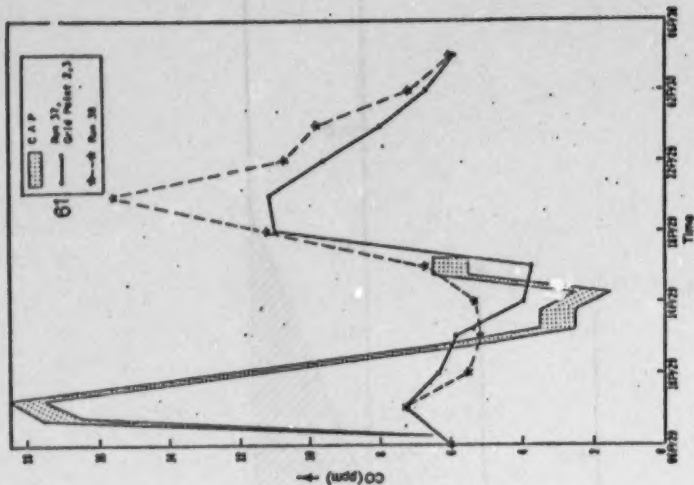
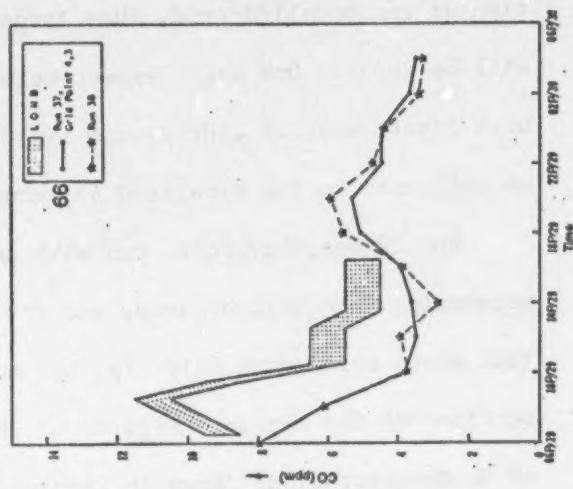
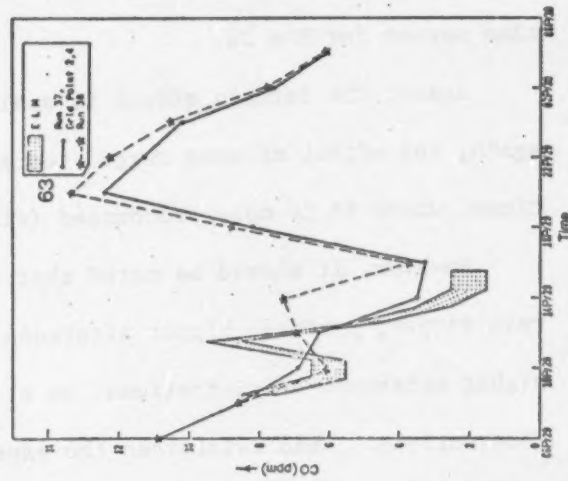
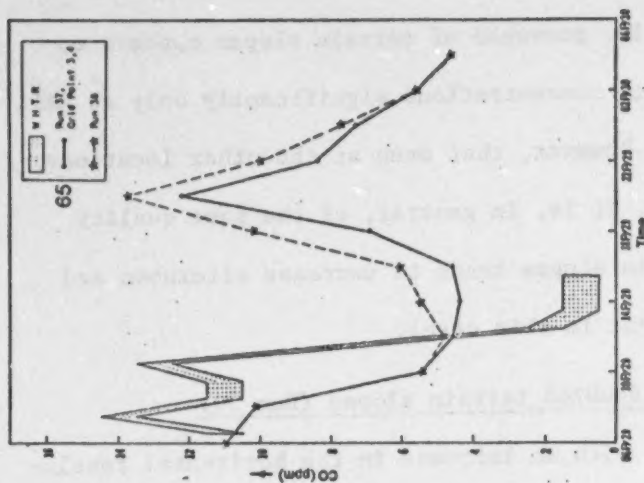
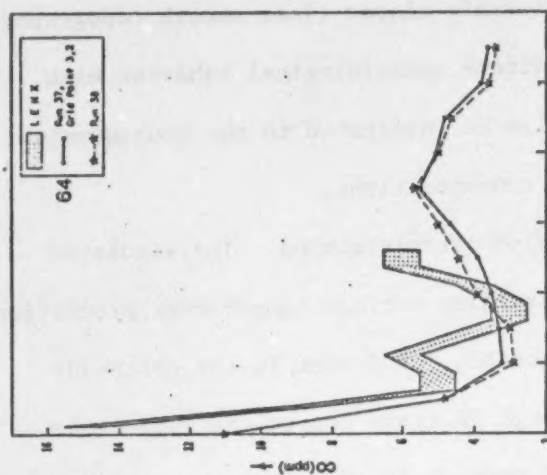
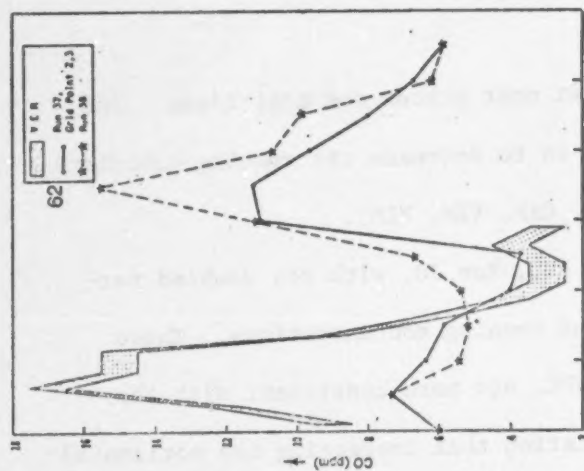


Figure 56. 06P/30 September. Vertical sections along the SW-NE diagonal of the modelled region showing simulated CO concentrations (ppm).



Figures 57 - 60. The time series of Figures 42 through 46 are repeated. Also shown are simulated time series for Run 38, in which the terrain slopes were set at zero everywhere in the modelled region.



Figures 61 - 66. The time series of Figures 47 through 51 are repeated. Also shown are simulated time series for Run 38, in which the terrain slopes were set at zero everywhere in the modelled region.

first, that the terrain effects are minor at most locations during the morning and early afternoon hours. The presence of terrain slopes appears to decrease the afternoon and evening concentrations significantly only at CAP, VER, and AZU. It is noteworthy, however, that even at the other locations where the effect is much smaller, it is, in general, of the same quality (viz., the presence of the terrain slopes tends to decrease afternoon and evening concentrations of pollutant in this case).

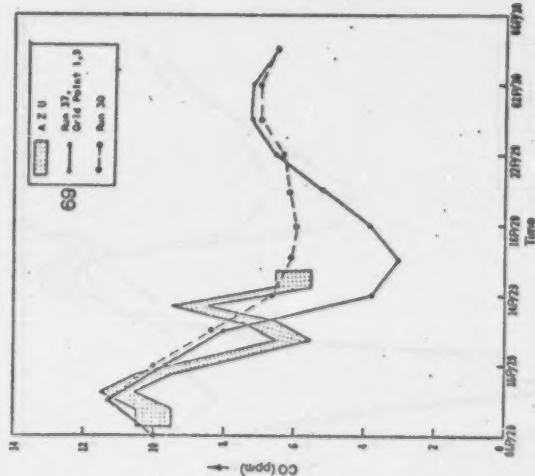
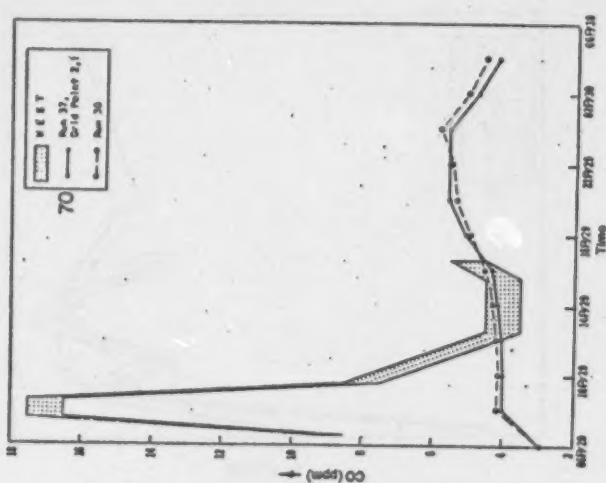
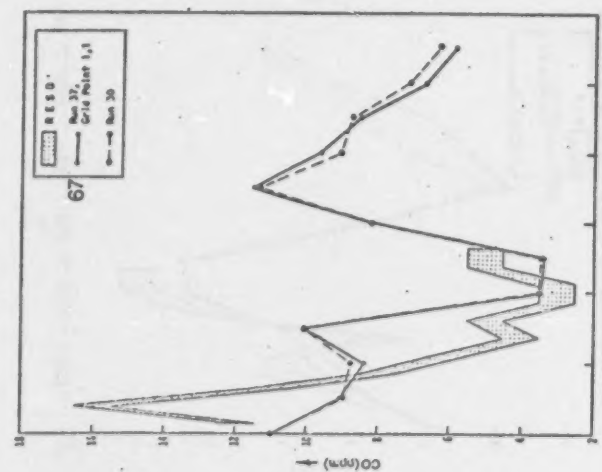
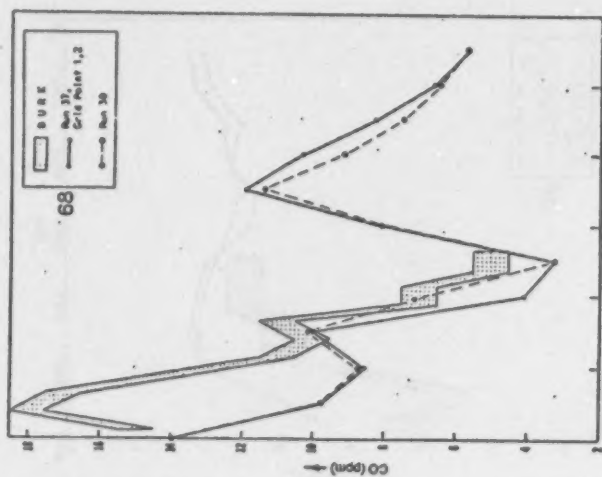
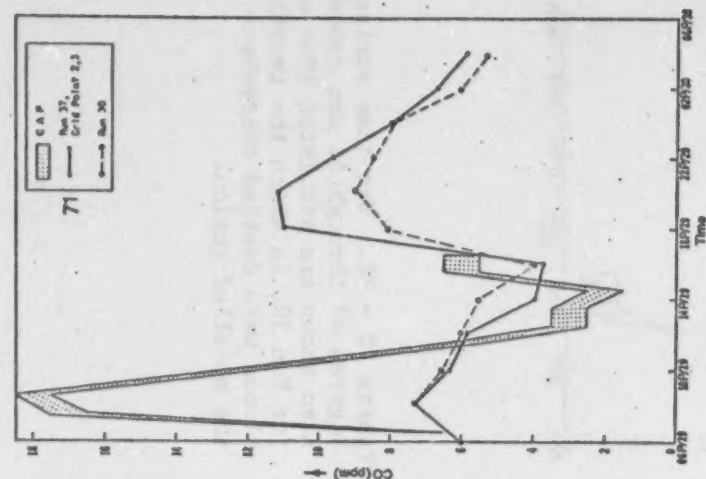
3.3.2.2 A simulation with doubled terrain slopes (Run 30)

It is reasonable to expect, with an increase in the horizontal resolution of the modelled grid, that larger terrain slopes (less smooth topography) will be input. One might expect more extreme meteorological behavior with such input; and, of course, one might also be interested in the consequences as reflected in the simulated pollutant concentrations.

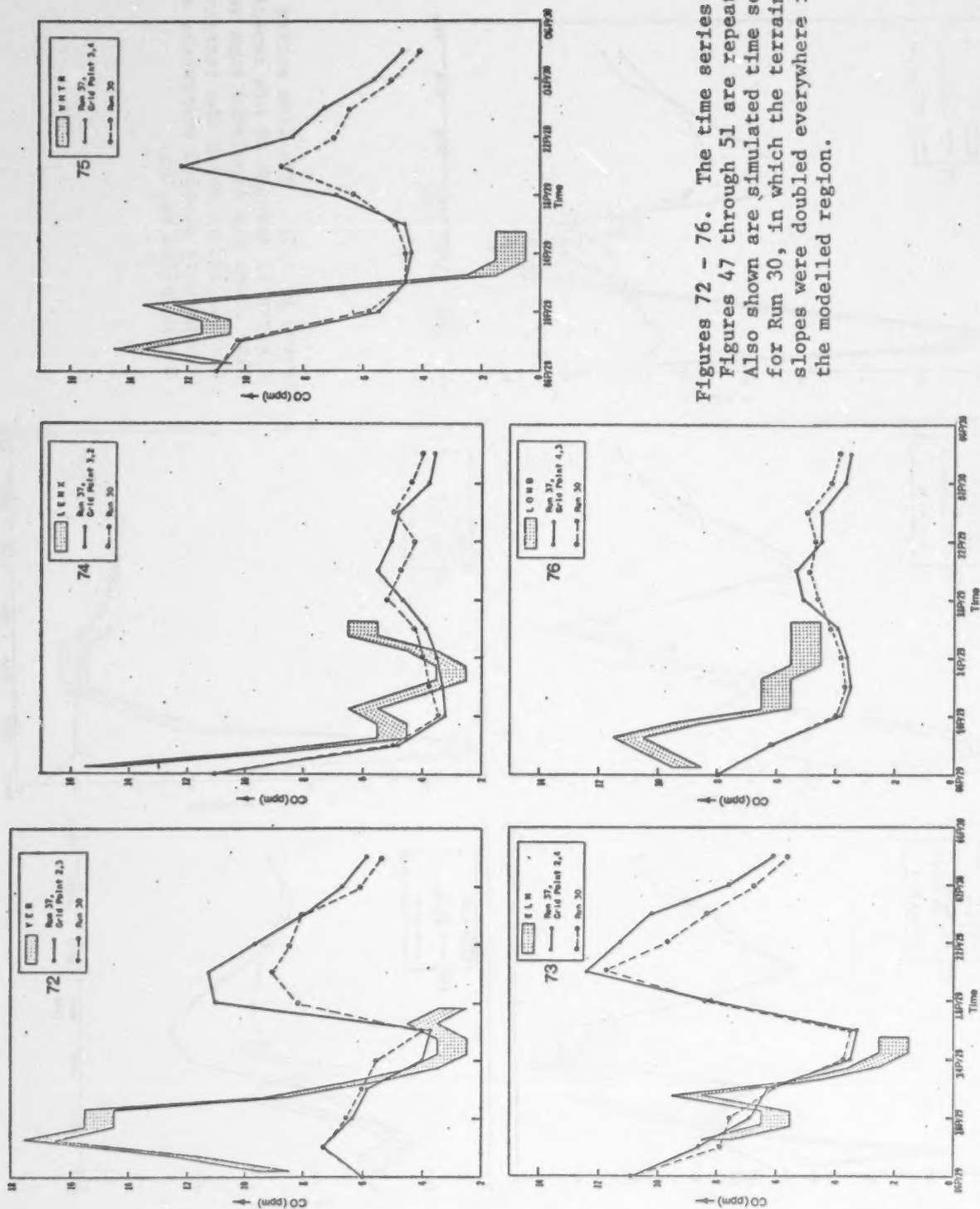
Run 30 was, therefore, run with doubled terrain slopes. The simulated meteorology was well behaved, and the resulting surface temperature predictions (not shown here) were slightly, but noticeably, different in the northeast portions of the region. Figures 67 through 76 again repeat the time series of CO concentrations shown in Figures 42 through 51, but also show simulated time series for Run 30.

Again, the terrain effect is small at most places and most times. And again, the effect of more rugged terrain is to decrease the evening concentrations, where it is more pronounced (viz., CAP, VER, ELM).

However, it should be noted that at AZU, Run 30, with the doubled terrain slopes, produces higher afternoon and evening concentrations. These higher afternoon concentrations, as at BURK, are more consistent with the observations. This reinforces the expectation that increasing the horizontal grid resolution, with a consequent increase in the resolution of the terrain



Figures 67 - 71. The time series of Figures 42 through 46 are repeated. Also shown are simulated time series for Run 30, in which the terrain slopes were doubled everywhere in the modelled region.



Figures 72 - 76. The time series of Figures 47 through 51 are repeated. Also shown are simulated time series for Run 30, in which the terrain slopes were doubled everywhere in the modelled region.

slopes, will lead to more accurate simulations.

3.3.3 Sensitivity of the Results to Other Modelling Changes

3.3.3.1 A simulation with the free atmospheric $K_{\min} = 10^4 \text{ cm}^2/\text{sec}$ (Run 39)

Figures 77 through 81 repeat the distributions of observed low-level CO concentrations at two hourly intervals, and the simulated patterns of CO concentration at the 4 m grid level obtained in the base run (37). Also shown in these figures are the changes in simulated values obtained in each grid cell by increasing the free atmospheric value of $K_{\min}$ to $10^4 \text{ cm}^2/\text{sec}$.

It is evident from these maps that this modelling change had, in general, an insignificant effect on the accuracy of the simulated concentrations, during the period for which validation measurements were available.

3.3.3.2 A simulation with doubled terrain slopes and $K_{\min} = 10^4 \text{ cm}^2/\text{sec}$ (Run 26)

Figures 82 through 86 also repeat the maps of observed and base run simulated CO concentrations first shown in Figures 37 through 41. Also shown on these maps are the changes in simulated values obtained with the simultaneous change of two modelling parameters which were changed individually in Runs 39 and 30 described above. The results are as would be expected from the results of the individual runs. However, it is more easily seen on these maps that the improvement in simulation accuracy obtained by using less smooth terrain slopes is confined to the northern boundary of the modelled region as might be expected.

Less easily explained is the fact that this improvement is apparent only in the early afternoon.

Figure 77. 08P/29 September

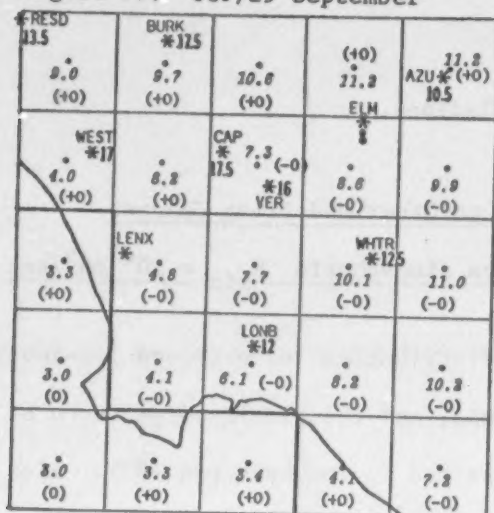


Figure 78. 10P/29 September

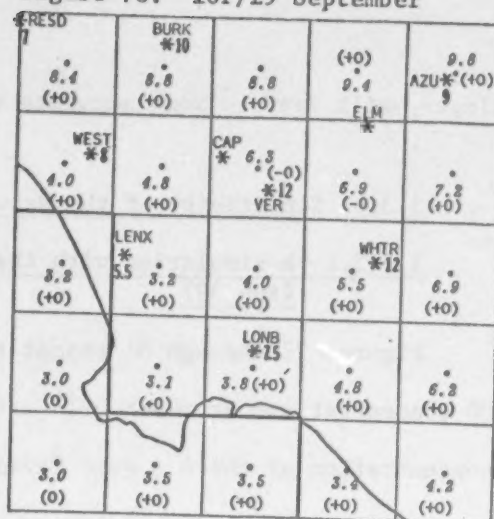


Figure 79. 12P/29 September

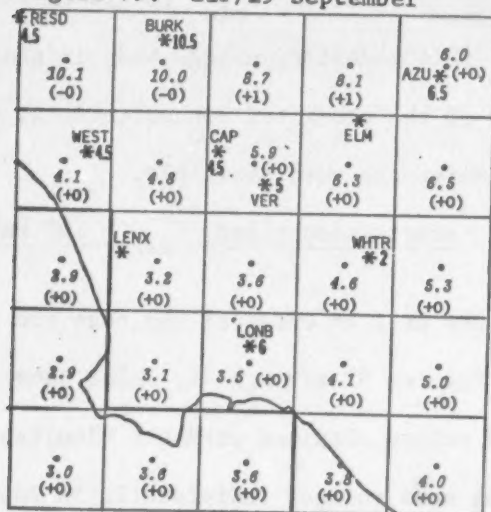


Figure 80. 14P/September

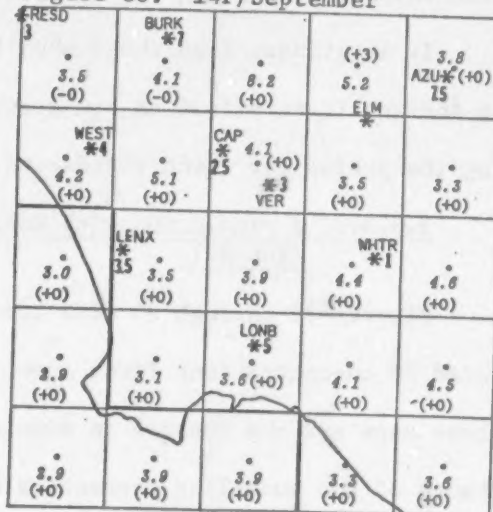
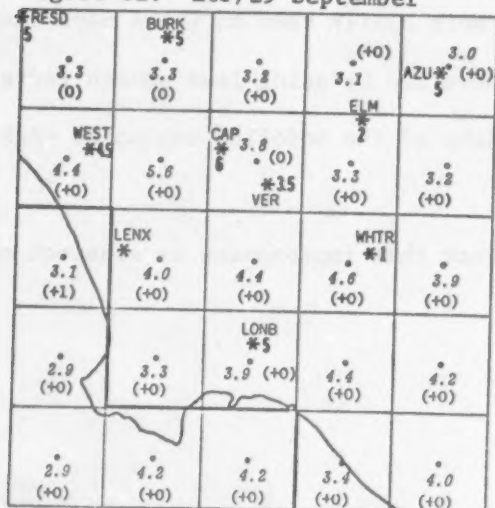


Figure 81. 16P/29 September

**Key**

- * CO Monitoring Station
- 15 Observed CO Concentrations at Station
- 9.8 CO Concentrations Predicted by Base Run 37
- (0) Change in CO Concentration for Run 39

Figures 77 - 81. The maps of Figures 37 through 41 are repeated. Also shown are changes in simulated CO concentrations induced in Run 39, in which the free atmospheric minimum diffusivity was increased to $10^4 \text{ cm}^2/\text{sec}$.

Figure 82. 08P/29 September

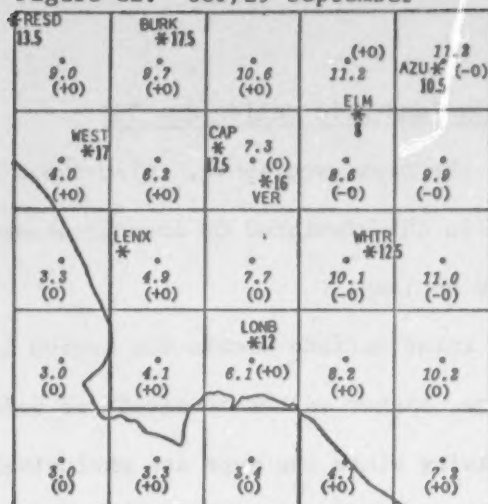


Figure 83. 10P/29 September

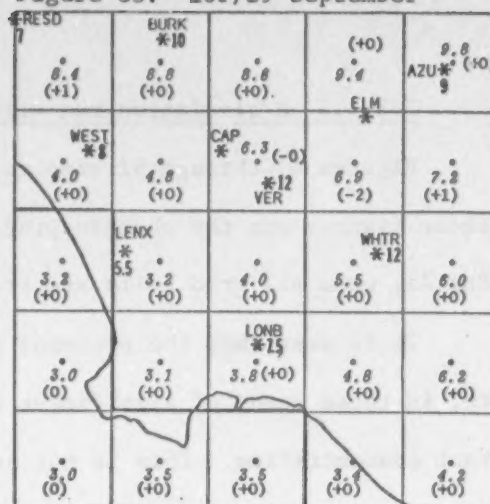


Figure 84. 12P/29 September

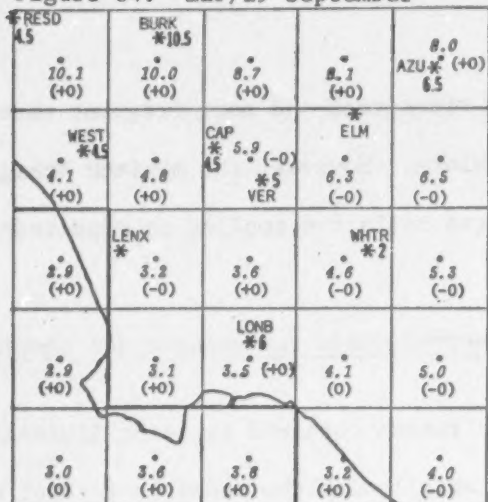


Figure 85. 14P/29 September

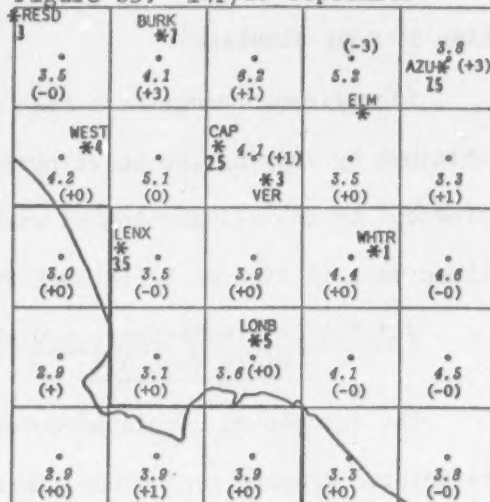
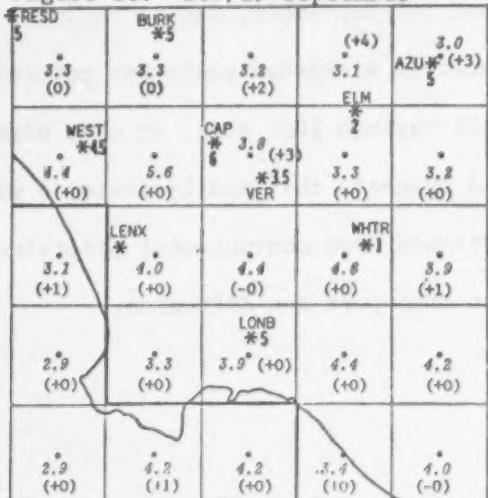


Figure 86. 16P/29 September

**Key**

- * CO Monitoring Station
- 3.3 Observed CO Concentrations at Station
- 8.8 CO Concentrations Predicted by Base Run 37
- (0) Change in CO Concentration for Run 26

Figures 82 - 86. The mpas of Figures 37 through 41 are repeated. Also shown are changes in simulated CO concentrations induced in Run 26, in which the terrain slopes were doubled and the minimum diffusivity were changed simultaneously.

3.3.3.3 A simulation run with only land grid cells (Run 33)

Figures 87 through 91 also repeat the maps used above. Also shown in these figures are the changes produced in the simulated CO concentrations of Run 33, when all grid cells are treated as land.

It is seen that the presence of a water surface within the region leads to, in those cases of significant change, higher values of simulated pollutant concentration. This is not surprising since the maps are exclusively for daylight hours, and one would expect the presence of water to lead to increased stability in the lower atmospheric layers during the day for the time of year simulated.

Significant changes are both more widespread and more frequent than those obtained by varying the input terrain slope. However, the maximum changes produced by the elimination of water grid cells are smaller in magnitude than those seen in Figures 82 through 86.

3.3.3.4 A simulation run with observed winds replacing model simulated winds (Run 31)

The changes in simulated CO concentration obtained by using linearly interpolated ground-level winds, instead of allowing the model to predict winds, are shown in Figures 92 through 96.

Only the first two maps, for 08P and 10P/September, show a definite, though minor, tendency toward more accurately simulated pollutant concentrations. The later maps in the series (12P through 16P) show, in many places, a decrease in simulation accuracy. This suggests that model-simulated winds may be at least as suitable as winds obtained from conventional observing networks for the prediction of pollutant transport and diffusion.

Figure 87. 08P/29 September

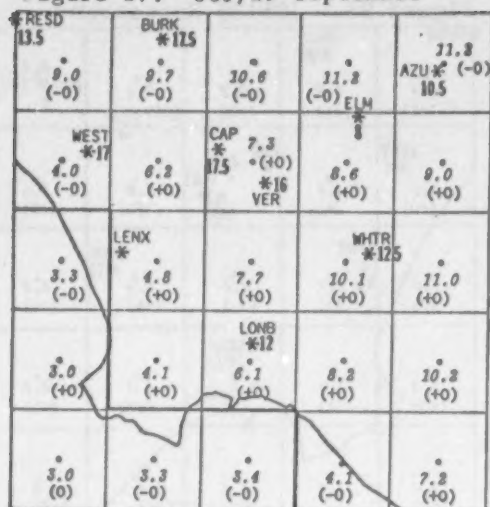


Figure 88. 10P/29 September

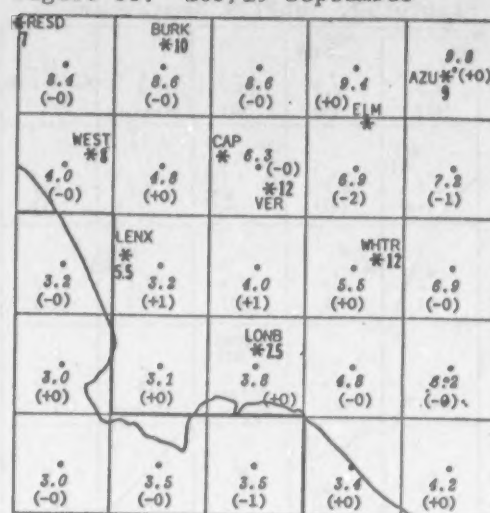


Figure 89. 12P/29 September

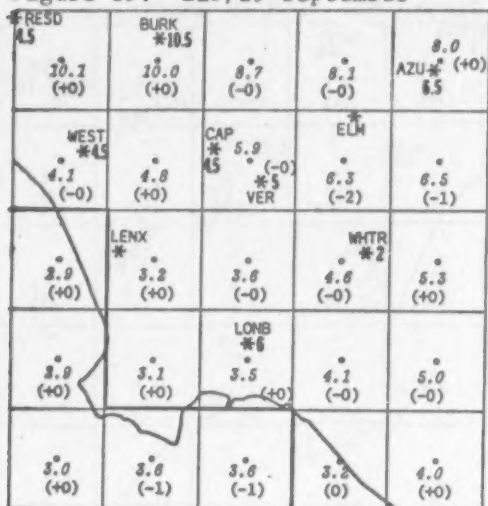


Figure 90. 14P/29 September

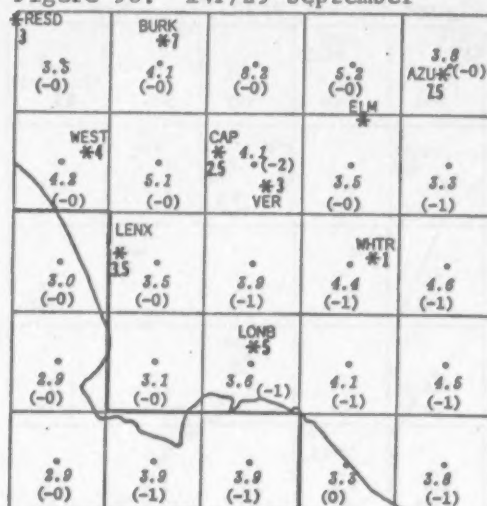
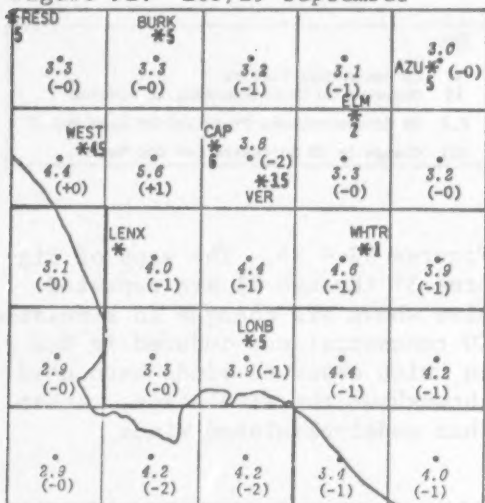


Figure 91. 16P/29 September



Key

- * CO Monitoring Station
- 9.8 Observed CO Concentrations at Station
- 9.8 CO Concentrations Predicted by Base Run 37
- (0) Change in CO Concentration for Run 33

Figures 87 - 91. The maps of Figures 37 through 41 are repeated. Also shown are changes in simulated CO concentrations induced in Run 33, in which all horizontal grid cells were designated as containing a land-air interface.

Figure 92. 08P/29 September

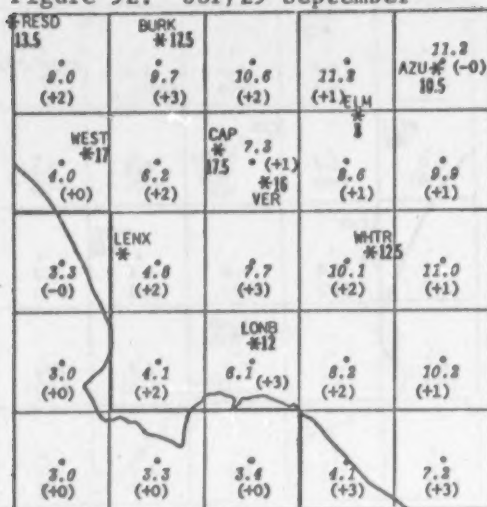


Figure 93. 10P/29 September

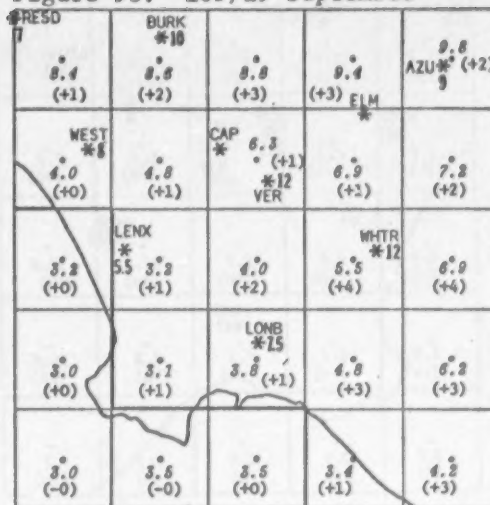


Figure 94. 12P/29 September

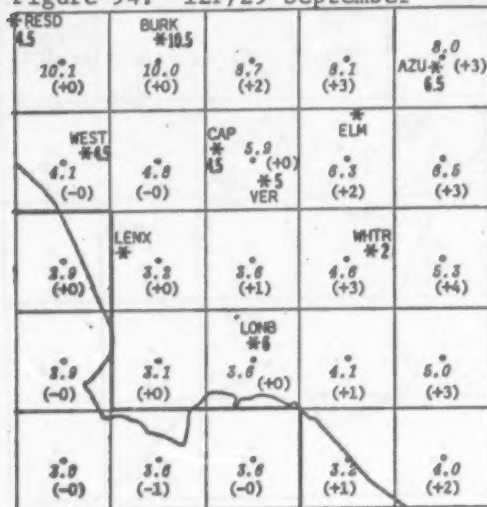


Figure 95. 14P/29 September

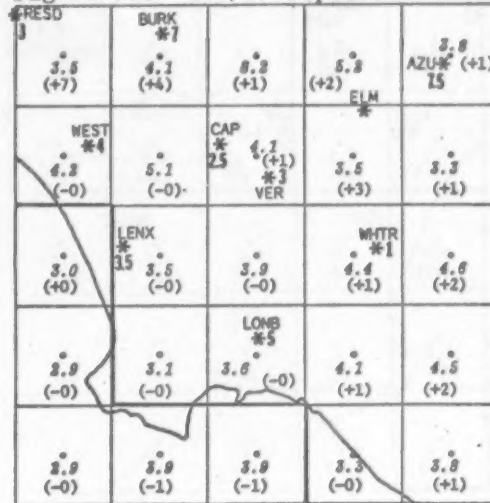
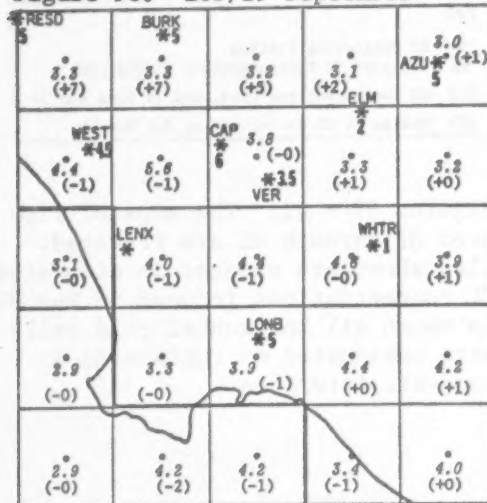


Figure 96. 16P/29 September



Key

- * CO Monitoring Station
- 3.8 Observed CO Concentrations at Station
- 3.8 CO Concentrations Predicted by Base Run 37
- (0) Change in CO Concentration for Run 31

Figures 92 - 96. The maps of Figures 37 through 41 are repeated. Also shown are changes in simulated CO concentrations induced in Run 31, in which observed winds were used throughout the simulation, rather than model-simulated winds.

3.3.3.5 A simulation run with increased soil moisture parameter (Run 19)

The changes in simulated CO concentration obtained by using an increased surface moisture index over the land areas are shown in Figures 97 through 101.

The most widespread and largest changes appear in the earliest maps. These changes decrease the simulation accuracy significantly.

3.3.4 Comparison with the Results of Other Models

A previously described model (Roth et al., 1971), applied to the same observational period, differs from the model used here in three major respects. First, the three-dimensional winds and diffusivities are input to Roth's model, and are obtained from analysis of data observed throughout the simulation period. Second, a finer and more extensive horizontal grid was used by Roth et al. (see Figure 2). Third, the source distributions for CO used by Roth, besides being defined on the finer grid (and presumably capturing more of the detail in vehicular traffic patterns), also include the regional airports in the source patterns. While these make a minor contribution to the region's total CO inventory, they may be locally and sporadically important in producing major variations.

We omitted the airport sources in the simulations described here on the assumption that their contribution would be minor as long as the coarse horizontal grid was used. This was borne out by a test simulation (not described elsewhere in this report) in which the airport sources were included with their contributions spread over the individual 64 square-mile grid cell in which each is located. The simulated concentrations were essentially the same as those shown for Run 37.

Figure 97. 08P/29 September

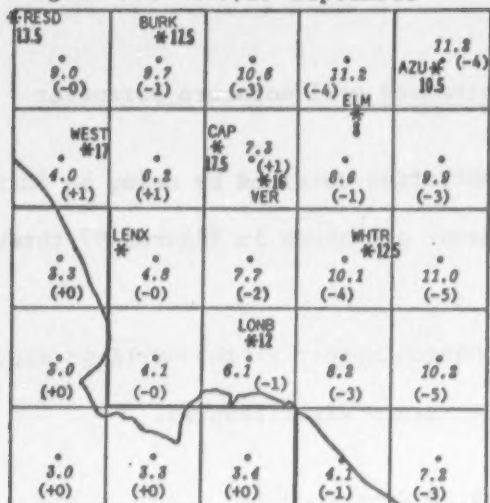


Figure 98. 10P/29 September

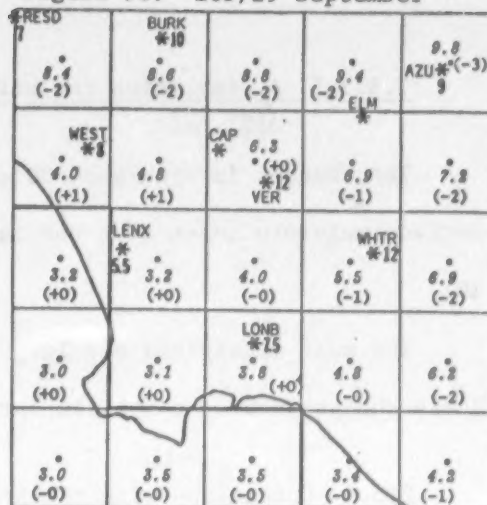


Figure 99. 12P/29 September

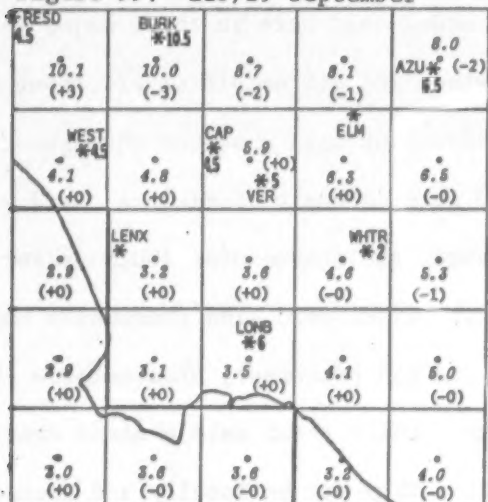


Figure 100. 14P/29 September

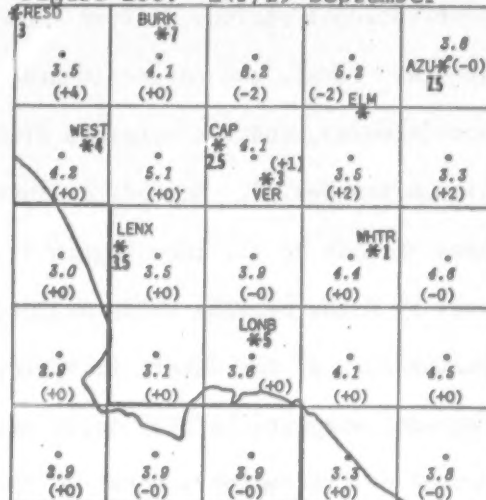
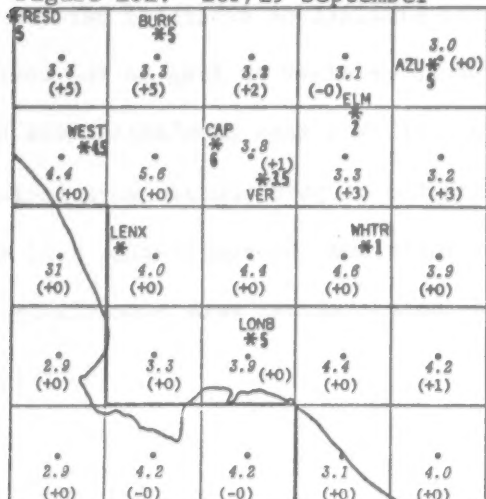


Figure 101. 16P/29 September

**Key**

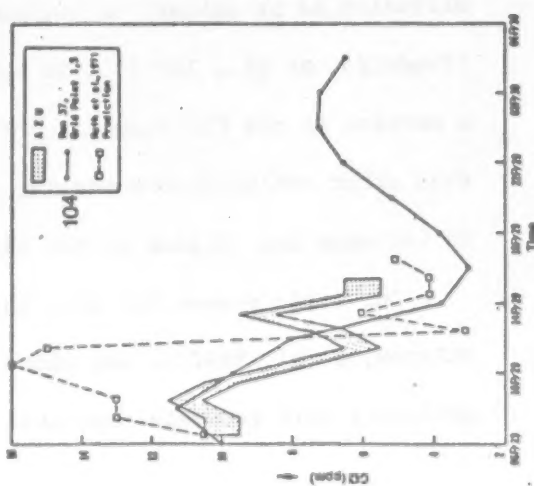
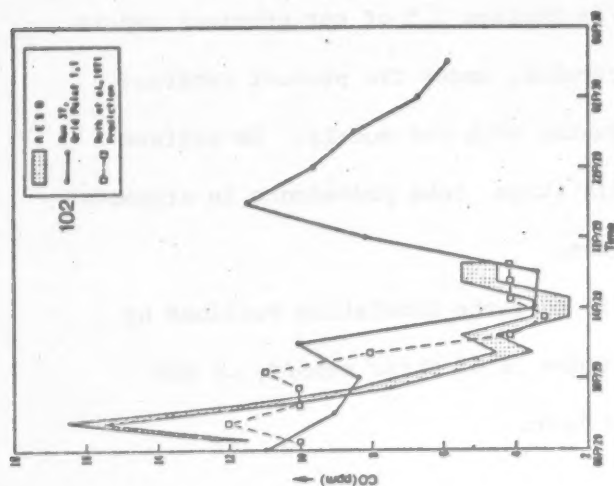
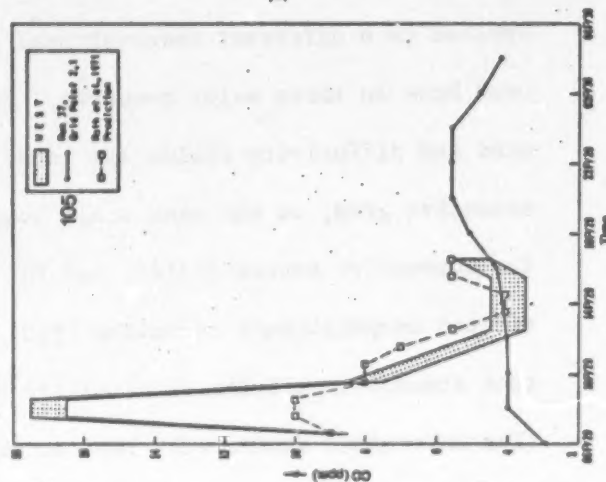
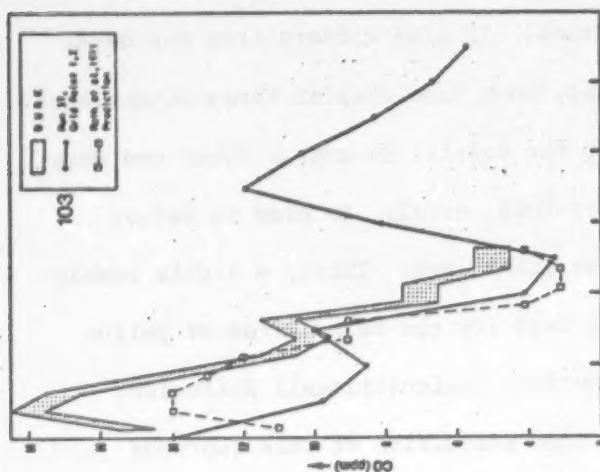
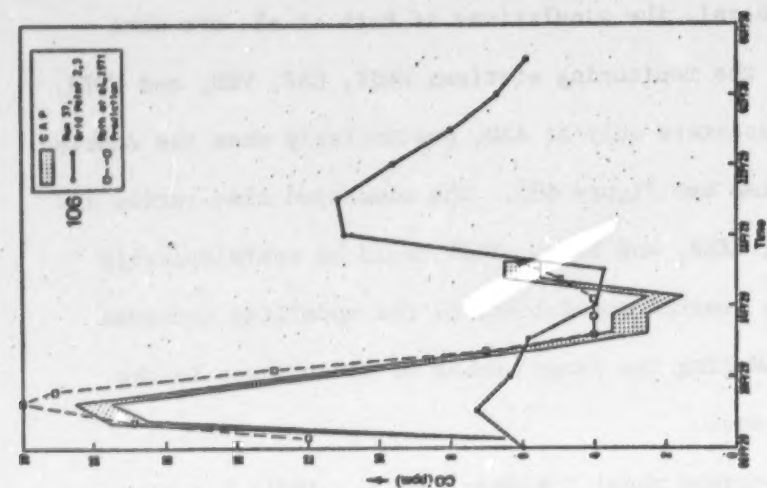
- * CO Monitoring Station
- 9.8 Observed CO Concentrations at Station
- 9.8 CO Concentrations Predicted by Base Run 37
- (0) Change in CO Concentration for Run 19

Figures 97 - 101. The maps of Figures 37 through 41 are repeated. Also shown are changes in simulated CO concentrations induced in Run 19, in which the surface moisture parameter was increased to 0.2 in all land grid cells of the model.

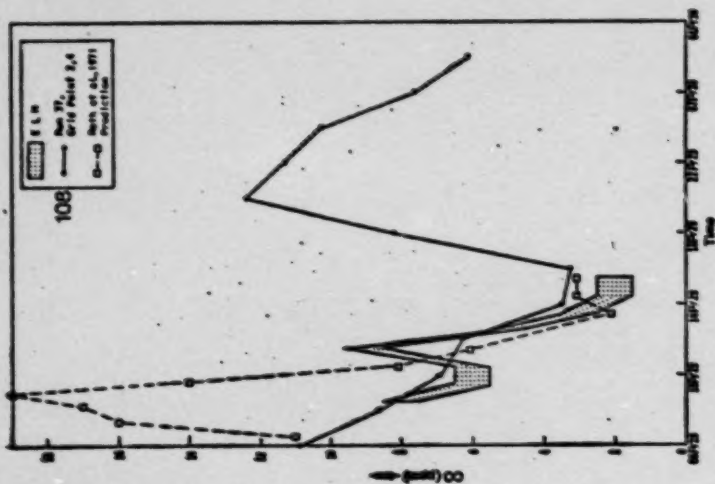
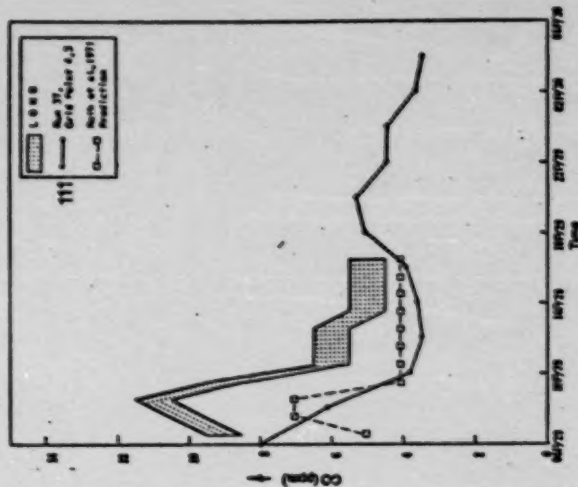
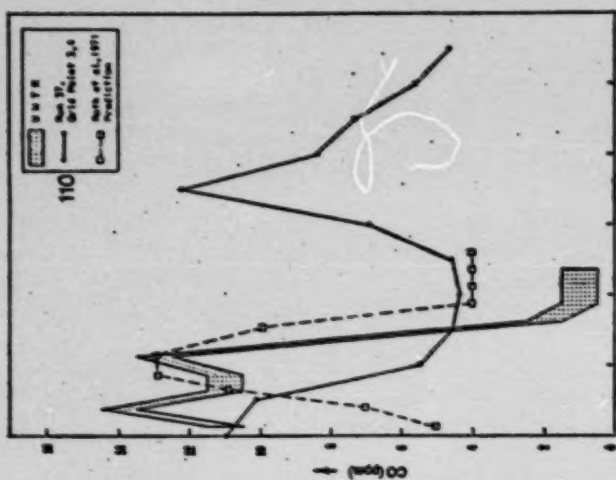
Figures 102 through 111 repeat the time series originally shown in Figures 42 through 51, but also show time series simulated by the model of Roth et al. (1971). In general, the simulations of Roth et al. are more accurate, particularly for the monitoring stations WEST, CAP, VER, and WHTR. Our model is clearly more accurate only at AZU, particularly when the doubled terrain slopes are used (also see Figure 69). The simulated time series are remarkably similar at RESD, LENX, and LONB. This could be optimistically interpreted in terms of the general consistency of the modelling concepts used in these models, considering the large number of differences in the detailed modelling assumptions.

Another previously described model (Sklarew, et al., 1971) has been applied to a different observational period. It also differs from the model used here in three major respects. First, much less complex three-dimensional wind and diffusivity fields are input to the model. Second, a finer and more extensive grid, on the same scale used by Roth, et al., is used to define the automotive source fields, and for the prediction. Third, a highly sophisticated computational technique (PIC) is used for the calculation of pollutant transport in order to eliminate numerical (calculational) diffusion. (The interested reader will find an extended discussion of this spurious diffusion as it appears in our models in Section 2.5 of our previous report [Pandolfo, et al., 1971]). We have prepared, under the present contract, a version of the PIC formulas for inclusion with our models. We believe that other modifications should, at this stage, take precedence in attempts to increase the realism of the simulation.

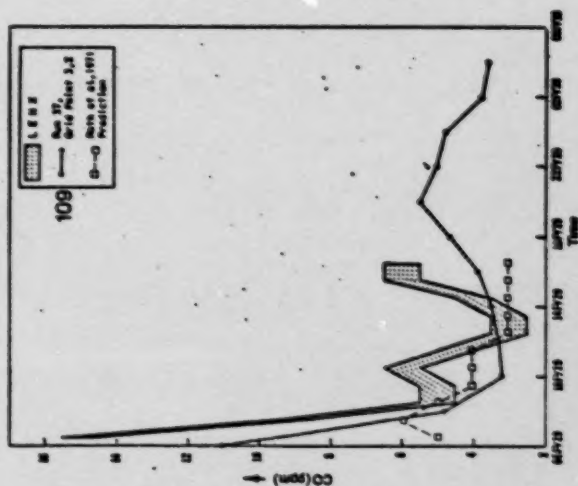
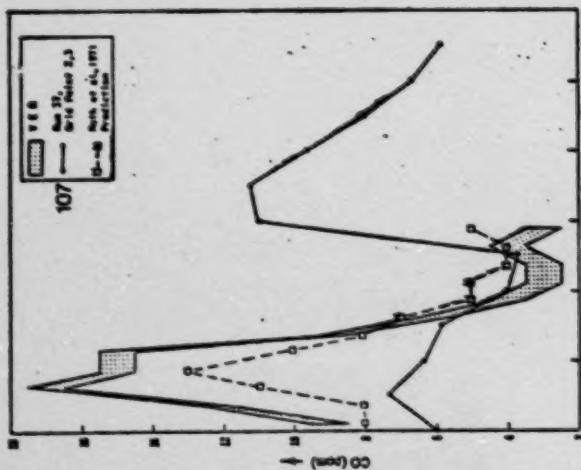
Our basic reason for this belief is that the simulation outlined by Sklarew, et al. (1971), and shown in Figure 31 of their report, is not obviously more accurate than that shown here.



Figures 102 - 106. The time series of Figures 42 through 46 are repeated. Also shown are simulated time series obtained by Roth et al. (1971).



Figures 107 - 111. The time series of Figures 47 through 51 are repeated. Also shown are simulated time series obtained by Roth et al. (1971).



4.0 SUMMARY AND CONCLUSIONS

The urban boundary-layer model described in a previous report (Pandolfo, et al., 1971) was modified and used in test runs to estimate the degree to which observed spatial and temporal variations of meteorological conditions and concentrations of a stable air pollutant within a complex urban region can be realistically simulated.

The major modification relevant to this project was the inclusion of an average terrain slope vector for each grid square in the input to the model. This slope is used to calculate topographically induced vertical velocity and its effects on the temperature, humidity, and pollutant within the region. The modelling equations, as modified, are presented. A series of simulations was conducted on a data base obtained from the results of observation projects at Los Angeles, California, on September 29-30, 1969. Forty full test simulations were run over the span of a few months. The observed meteorological parameters form a sparse set of data in the four-dimensional (space-time) mesh needed to define the relevant meteorology for this application. Many of the runs varied the meteorological input about the standard (observed) set. It has, therefore, been demonstrated that an economical, objective, physically consistent, and precisely specified (though with some arbitrary elements) procedure has been achieved for obtaining and predicting the three-dimensional meteorological fields needed. This procedure provides a necessary supplement to the pollutant transport-diffusion portion of the model developed here; or to other pollutant models developed elsewhere. Heretofore, these other models (e.g., Sklarew, et al., 1971; Eschenroeder and Martinez, 1971; and Roth, et al., 1971) have relied on incomplete meteorological fields subjectively and laboriously obtained, that are difficult to generalize to other weather situations. In several of the runs the input

topography, land-water distribution, and other physical characteristics of the underlying surface was varied. The results demonstrate that ready generalization to other regions can be expected.

For purposes of economy in these initial tests, and for reasons of physical consistency, a major simplification was made, and the modelled region is simulated on a relatively coarse 5x5 horizontal grid with 8-mile grid spacing. This is in contrast to other models which focus on the prediction of pollutants only, and which are based on finer horizontal grids with 2-mile grid spacing (Sklarew, et al., 1971; Roth, et al., 1971). Nonetheless, the temporal and spatial variations of those meteorological conditions for which observations are available, via., air temperature, humidity, and wind, are simulated with an encouraging degree of realism. Temporal and spatial variations of CO are also simulated fairly realistically, with somewhat less accuracy than in the model described by Roth, et al. (1971), and with accuracy equivalent to that shown by Sklarew, et al. (1971). It is reasonable to expect improved simulation accuracy with the finer horizontal resolution used in these other models, and the performance of such simulations with this model is strongly urged.

Slight differences of simulation accuracy of surface-layer CO concentrations are seen when the model is modified to neglect the presence of the ocean, to neglect the terrain slope, and to increase the soil moisture parameter. On balance, these changes appear to decrease the simulation accuracy.

More significant increases of simulation accuracy at two of the stations in the vicinity of the San Gabriel Mountains in the early afternoon, are obtained when the smoothed terrain slopes are doubled in magnitude. This reinforces the expectation of improved simulation accuracy with a finer grid, and, consequently, less smoothing of the topographic features.

Noticeable changes in simulation accuracy are seen when observed winds are used to circumbent the model prediction of wind. The increases in accuracy at some stations and times appear to be balanced by decreases in accuracy at other stations and times.

Insignificant changes in simulation accuracy are seen when the minimum free atmospheric value of diffusivity is increased by an order of magnitude.

A major deficiency of the simulated CO variations is the underestimation of morning peak concentrations in the earliest stages of the simulation at many horizontal locations. A similar deficiency was noted in the model simulations of Sklarew, et al. (1971) and was eliminated by modification of the modelled vertical distribution of vertical eddy diffusivity in that study. The model of Roth, et al. (1971) does not exhibit this deficiency, but does overestimate morning peak concentrations at other stations.

Before other measures to eliminate this deficiency are investigated, a test simulation should be performed with the refined grid (2x2 mile) as used in other models, and with the addition of airports to the source inventory.

This is expected to yield the greatest improvement in accuracy (through the more detailed definition of the emission sources and topography) at no development cost, with only increased, and easily bearable, computer costs added.

Other recommended changes, in order of decreasing priority, are:

- 1) inclusion of additional reactive pollutants along with their associated photochemical formulations (e.g., as outlined in Roth, et al., 1971);
- 2) generalization to a non-hydrostatic formulation (see Appendix D);
- 3) the inclusion of a (numerically) more accurate differencing scheme for the horizontal transport with explicit treatment of the horizontal diffusion (see Appendix E); and

- 4) optimization of the computer program to eliminate details that are superficially unnecessary in this application, e.g., the requirement to carry as many grid levels in the soil as are needed in the water portions of the model.

Implementation of item (1), according to rough estimates based on Roth, et al. (1971) and Sklarew, et al. (1971), would increase the running time by an order of magnitude. However, such time, and the cost implied, is feasible for the full range of applications in air quality simulation on more advanced computers for which the model is intended than the IBM 360/65 used in this project. Relative to this increase, the increases (or savings) in computational costs resulting from the implementations of items (2), (3), and (4) become trivial. The development of the necessary formulations for (2) and (3) have been carried out (Appendices D and E). In this context, it is our opinion that the kinds of programming changes that might be carried out under (4), though superficially appealing on aesthetic grounds, and easily implemented, should take on the lowest priority.

In summary, we present here what is to our knowledge the only documented and validated three-dimensional model. We know of no other model that has achieved multi-day predictions or simulations of both meteorological variables and conservative pollutants on the spatial scales considered here. As is inherent in any complex model, there are apparent variations in the degree of accuracy of treatment of the many processes and parameters included in both the input and formulation. It is, however, unreasonable to expect agreement among scientists as to exactly which components are treated too crudely, and which are treated too accurately, until much more experience has been gained with the model. It has also been demonstrated that many useful results can be provided in this application while this experience is being gained.

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6.0 ACKNOWLEDGEMENTS

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The University of Connecticut Computer Center contributed significantly more, in computer time, than the computer project budget.

Appendix A

Specifications for the Computer Program

A.1 Introduction

The purpose of this section is to describe the set of finite-difference equations which are solved in the computer program. These equations are the analogues of simplified forms of the prognostic differential equations (see Section 2.0) for various scalar properties in the planetary boundary layer of the atmosphere, ocean, and soil system. The scalar properties include wind and current components, temperature, specific humidity, salinity, and pollutants. The units of specific humidity and salinity in this section are g/kg rather than g/g as in Section 2.0. Much of these specifications is based on the specifications and modifications in the Appendices to Pandolfo et al. (1971).

The upper and lower boundary values required for the numerical solutions of the equations are to be input or computed from input. The equations are to be solved on a specified, arbitrarily spaced, vertical mesh, which is also input. Figure A is a schematic diagram of a vertical grid mesh. This figure should provide the reader with a better understanding of the indexing necessary for the presentation of the finite-difference equations. The two vertical grid points associated with the interface represent the air and land (water) sides of the interface.

Volume II of this report contains the FORTRAN program listings for all the subroutines and flow diagrams for the MAIN program of both versions (RIGID LID and FREE SURFACE) of the model.

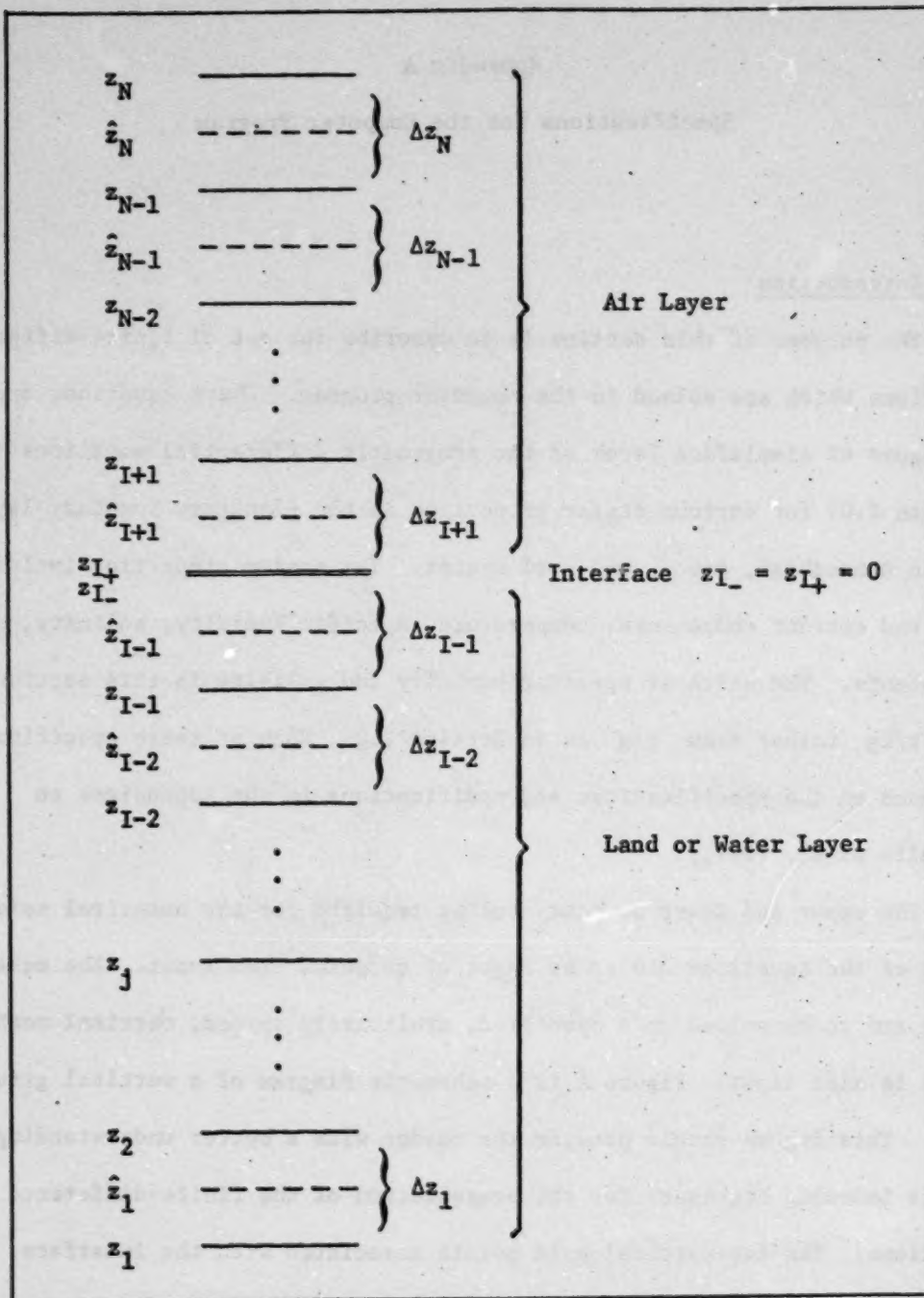


Figure A. Schematic diagram of vertical grid mesh.

A.2 Input

The input is specified either for the entire grid, for one location in the grid, or for each station of the grid. Input specifications for both versions of the model are contained in Volume II.

A.3 List of Additional Symbols

A.3.1 General Parameters

I_+	Number of vertical grid levels from the bottom of the boundary layer to the air side of the interface.
I_-	Number of vertical grid levels from the bottom of the boundary layer to the water or soil side of the interface.
$J_{\max}$	Number of stations in the x-direction.
$K_{\max}$	Number of stations in the y-direction.
N	Number of vertical grid levels within the boundary layer.
z_g	Heights of input gradients (cm).
ZW	Height of vertical grid level used in computation of wave dimensions (cm). This height is 1950 cm or the lowest grid level above 1950 cm.
Δ	Horizontal grid length.
ϵ_s	Infrared emissivity of surface.

A.3.2 General Grid Location

j_0, k_0	The horizontal grid indices corresponding to the x,y locations (respectively) of the input initial vertical profiles of the dependent variables.
$P_1(z_j, 0)$	Initial values of Pollutant 1 (g/100 g); $z_{I+} < z_j \leq z_N$.
$P_2(z_j, 0)$	Initial values of Pollutant 2 (g/100 g); $z_{I+} < z_j \leq z_N$.
$q(z_j, 0)$	Initial values of specific humidity (g/kg); $z_{I+} < z_j \leq z_N$.
$s(z_j, 0)$	Initial values of salinity (g/kg); $z_1 \leq z_j \leq z_{I-}$.
$T(z_j, 0)$	Initial values for temperature ($^{\circ}K$); $z_1 \leq z_j \leq z_N$.

- $u(z_j, 0)$ Initial values of eastward velocity components (cm/sec),
 $z_1 \leq z_j \leq z_N$.
- $v(z_j, 0)$ Initial values of northward velocity components (cm/sec),
 $z_1 \leq z_j \leq z_N$.

A.3.3 Input at Each Station

- h_{1i}, h_{2i} Fractional strength of emission for pollutants 1 and 2 at the i (th) height level.
- $K_T(\hat{z}_j)$ Soil thermal conductivity for each soil layer (cm²/sec),
 $\hat{z}_j < 0$.
- n_g Number of geostrophic wind and current input values.
- $S_1(t)$ Source strength for pollutant 1 ($\mu\text{g}/\text{m}^2$).
- $S_2(t)$ Source strength for pollutant 2 ($\mu\text{g}/\text{m}^2$).
- $U_g(z_{I-}, t)$ Eastward components of the geostrophic current at the interface (cm/sec).
- $V_g(z_{I-}, t)$ Northward components of the geostrophic current at the interface (cm/sec).
- $U_g(z_N, t)$ Eastward components of the geostrophic wind at the upper boundary (cm/sec).
- $V_g(z_N, t)$ Northward components of the geostrophic wind at the upper boundary (cm/sec).
- ρ_s Density of soil (g/cm³).

A.3.4 Computations of Program Constants

$$\bar{c} = 3(R_c)^{1/3}(1 + R_c)^2$$

$$c_a = .239$$

$$c_w = .935$$

$$C = 3k^{4/3}h^{-2/3}$$

$$f = 14.585 \sin \phi \times 10^{-5}$$

$$g = 980$$

$$h = k^2(3/\bar{c})^{3/2}$$

$$k = .4$$

$$\begin{aligned}
k_1 &= .14 \\
n_T &= 3/2 \\
n_V &= 1/2 \\
R_c &= -1/7\alpha = .048 \\
\alpha &= -3 \\
\beta_T &= 10/3 \\
\beta_V &= 10 \\
\Gamma &= .98 \times 10^{-4} \\
\pi &= 3.1416 \\
\rho_a &= 10^{-4} \\
\rho_w &= 1 \\
\sigma &= 1.354 \times 10^{-12}
\end{aligned}$$

A.4 Parameters Constant Over Entire Grid

The height grid parameters are computed according to the notation

$$\hat{z}_j = \begin{cases} \left| \frac{z_j + z_{j+1}}{2} \right|, & j = 1, \dots, I-1 \\ \left| \frac{z_{j-1} + z_j}{2} \right|, & j = I+1, \dots, N \end{cases} \quad (58)$$

where $z_1 \leq z_j \leq z_N$, and the absolute value is used because depths that belong to the interface are taken to be negative. The value of $\hat{z}_I$ will always be zero since $z_{I-} = z_{I+} = 0$. The distance between vertical grid points is given by

$$\Delta z_j = \begin{cases} z_{j+1} - z_j, & j = 1, \dots, I-1 \\ z_j - z_{j-1}, & j = I+1, \dots, N. \end{cases} \quad (59)$$

The input horizontal gradients

$$\frac{\partial T}{\partial x}(z_j) ; \frac{\partial T}{\partial y}(z_j) \quad z_1 \leq z_j \leq z_N$$

$$\frac{\partial q}{\partial x}(z_j) ; \frac{\partial q}{\partial y}(z_j) \quad z_{I+} \leq z_j \leq z_N$$

$$\frac{\partial s}{\partial x}(z_j) ; \frac{\partial s}{\partial y}(z_j) \quad z_1 \leq z_j \leq z_{I-}$$

$$\frac{\partial u}{\partial x}(z_j) ; \frac{\partial u}{\partial y}(z_j) \quad z_1 \leq z_j \leq z_N$$

$$\frac{\partial v}{\partial x}(z_j) ; \frac{\partial v}{\partial y}(z_j) \quad z_1 \leq z_j \leq z_N$$

$$\frac{\partial P_1}{\partial x}(z_j) ; \frac{\partial P_1}{\partial y}(z_j) \quad z_1 \leq z_j \leq z_N$$

$$\frac{\partial P_2}{\partial x}(z_j) ; \frac{\partial P_2}{\partial y}(z_j) \quad z_1 \leq z_j \leq z_N$$

are to be computed through linear interpolation in the vertical at levels for which they are not specified. Linear interpolation is performed if more than one gradient of a dependent variable is input within a layer. If only one gradient changes at the interface, the input value is given at z_{I-} and z_{I+} for both the subsurface and the air. These gradients are independent of horizontal location and will be used at the horizontal grid boundary, whenever necessary.

A.5 Initial Profiles

The initial profile of the variables u, v, T, q, s, P_1 , and P_2 are computed from the input vertical profile at grid location j_0, k_0 . The initial profile ($t = 0$) of X_1 at horizontal grid point (j, k) and height n is computed from

$$(X_1)_{j,k}^n = (X_1)_{j_0,k_0}^n - \left(\frac{\partial X_1}{\partial y}\right)^n (k_0 - k)\Delta - \left(\frac{\partial X_1}{\partial x}\right)^n (j_0 - j)\Delta \quad (60)$$

where the gradients are the input gradients. For u , v , and T , the added restriction

$$(X_1)^{I-} = (X_1)^{I+} \quad (61)$$

is used. At each land station, a subsurface temperature profile is input for each station and the subsurface profiles of u , v , s , P_1 and P_2 are set to zero.

A.6 Eddy Exchange Coefficient

The eddy exchange coefficients are computed at each time step for each station. The subscript m is used to indicate eddy viscosity coefficients. Eddy conductivity-diffusivity is subscripted with e . Special formulas for the exchange coefficients at the $\hat{z}_{I-1}$ and $\hat{z}_{I+1}$ levels are given in Section A.10.

If the subsurface is water, a relevant wave property used to determine the mixing is the vertical gradient of the scalar value of the average orbital velocity in a turbulent wave. For a given non-zero λ and δ , this wave property, S_w , is given by

$$S_w(\hat{z}_j) = g^{\frac{1}{2}} \delta \left(\frac{\lambda}{2\pi}\right)^{-\frac{1}{2}} e^{-\hat{z}_j \cdot 2\pi/\lambda}, \quad (62)$$

where $\hat{z}_1 \leq \hat{z}_j \leq \hat{z}_N$. If no characteristic wavelength is specified (viz., $\lambda = 0$ for a water subsurface), δ is set equal to .055 and S_w is computed from the average wave height, $\bar{H}$, based on the formulas,

$$W(ZW, t) = [u^2(ZW, t) + v^2(ZW, t)]^{\frac{1}{2}} \quad (63a)$$

$$W(ZW_{-1}, t) = [u^2(ZW_{-1}, t) + v^2(ZW_{-1}, t)]^{\frac{1}{2}} \quad (63b)$$

$$W_{1950}(t) = W(ZW, t) \cdot A_1 + W(ZW_{-1}, t) \cdot A_2 \quad (63c)$$

where ZW_{-1} equals the vertical grid level immediately below ZW , and

$$A_1 = \frac{\ln 1950/ZW_{-1}}{\ln \frac{ZW}{ZW_{-1}}} \quad (64a)$$

$$A_2 = \frac{\ln \frac{ZW}{1950}}{\ln \frac{ZW}{ZW_{-1}}} \quad (64b)$$

From the wind speed at 1950 cm, the average wave height can be computed

$$\bar{H}(t) = 1.54165 \times 10^{-4} [W_{1950}(t)]^2 \quad (65)$$

Here S_w is computed:

$$\begin{aligned} S_w(\hat{z}_j, t) &= g^{\frac{1}{2}} \delta \left(\frac{\bar{H}}{\delta \cdot 2\pi} \right)^{-\frac{1}{2}} e^{-\hat{z}_j \cdot 2\pi \cdot \delta / \bar{H}} ; \bar{H} > 0 \\ &= 0 ; \bar{H} = 0 \end{aligned} \quad (66)$$

where $\hat{z}_1 \leq \hat{z}_j \leq \hat{z}_N$. To set a lower limit of the atmospheric exchange coefficient (see Section A.6.1.4), and for printout use, the average height of the 1/3 highest wave is computed by

$$H_{1/3}(t) = .8727 \times 1.5989 \bar{H}(t) \quad (67)$$

If the subsurface is land, $S_w(\hat{z}_j) = 0$ for $\hat{z}_1 \leq \hat{z}_j \leq \hat{z}_{I-1}$.

Coefficients used in the eddy exchange formulas are computed from one of the following sets of equations according to the value of λ ;

• for $\lambda \neq 0$;

$$\begin{aligned} K_0(\hat{z}_j) &= k^2 \left(\hat{z}_j + \frac{\delta\lambda}{2} \right)^2 ; \quad \hat{z}_{I+1} \leq \hat{z}_j \leq \hat{z}_N \\ K_0(\hat{z}_j) &= k_1^2 \left(\hat{z}_j + \frac{\delta\lambda}{2} \right)^2 ; \quad \hat{z}_1 \leq \hat{z}_j \leq \hat{z}_{I-1} ; \end{aligned} \quad (68)$$

• for $\lambda = 0$,

$$\begin{aligned} K_0(\hat{z}_j, t) &= k^2 \left(\hat{z}_j + \frac{\bar{H}}{2} \right)^2 ; \quad \hat{z}_{I+1} \leq \hat{z}_j \leq \hat{z}_N \\ K_0(\hat{z}_j, t) &= k_1^2 \left(\hat{z}_j + \frac{\bar{H}}{2} \right)^2 ; \quad \hat{z}_1 \leq \hat{z}_j \leq \hat{z}_{I-1} . \end{aligned} \quad (69)$$

A.6.1 The Atmospheric Layer ($\hat{z}_{I+2} \leq \hat{z}_j \leq \hat{z}_N$)

Note that the computed quantities S , L , $\bar{T}$, Ri , K_m , K_e are understood to be dimensioned variables with the coordinates $(\hat{z}_j, t)$:

$$S = \left\{ \left(\frac{u(z_{j+1}) - u(z_j)}{\Delta z_{j+1}} \right)^2 + \left(\frac{v(z_{j+1}) - v(z_j)}{\Delta z_{j+1}} \right)^2 \right\}^{\frac{1}{2}} \quad (70)$$

$$L = \left(\frac{T(z_{j+1}) - T(z_j)}{\Delta z_j} \right) + \Gamma + .00061 \bar{T} \left(\frac{q(z_{j+1}) - q(z_j)}{\Delta z_{j+1}} \right) \quad (71)$$

$$\bar{T} = \left(\frac{T(z_{j+1}) + T(z_j)}{2} \right) \quad (72)$$

$$Ri = \frac{g \cdot L}{\bar{T} [S + S_w(\hat{z}_j)]^2} , \quad Ri \leq \left| \frac{1}{\alpha} \right| . \quad (73)$$

If $\bar{T}(S + S_w) = 0$, check L ; if $L < 0$, go to A.6.1.3; if $L = 0$, set $R_1 = 0$; and if $L > 0$, set $R_1 = |1/\alpha|$. If $R_1 \geq 0$, proceed as in A.6.1.1; if $-.048 < R_1 < 0$, proceed as in A.6.1.2; if $R_1 \leq -.048$, proceed as in A.6.1.3.

A.6.1.1 If $R_1 \geq 0$

$$K_m = K_0(\hat{z}_j)[S + S_w(\hat{z}_j)][1 + \alpha R_1]^2 \quad (74a)$$

$$K_e = K_m \quad (74b)$$

and proceed to A.6.1.4.

A.6.1.2 If $-.048 < R_1 < 0$

$$K_m = K_0(\hat{z}_j)[S + S_w(\hat{z}_j)][1 - \alpha R_1]^{-2} \quad (75a)$$

$$K_e = \frac{K_m}{(1 - \alpha R_1)} \quad (75b)$$

and proceed to A.6.1.4.

A.6.1.3 If $-.048 \geq R_1$

$$K_e = \frac{h}{k^2} K_0(\hat{z}_j) \cdot \left| \frac{R \cdot L}{\bar{T}} \right|^{\frac{1}{2}} \quad (76a)$$

$$\begin{aligned} K_m &= K_e \cdot \left(\frac{3}{C} \right)^{-1/2} \cdot |R_1|^{-1/6} ; \bar{T}(S + S_w)^2 > 0 \\ &= 0 ; \bar{T}(S + S_w)^2 = 0, \end{aligned} \quad (76b)$$

and proceed to A.6.1.4.

A.6.1.4 Apply the limits

$$\begin{aligned} 10^4 &\leq K_{m,e} \leq 10^7 ; \hat{z}_j \geq 10^4 \\ \Lambda &\leq K_{m,e} \leq 10^7 ; \hat{z}_{I+1} \leq \hat{z}_j \leq 10^4, \end{aligned}$$

where $\Lambda = \lambda^2 = z_0^2$ for a land subsurface, or $\Lambda = (H_{1/3})^2$ for a water surface.

A.6.2 The Oceanic Layer ($\hat{z}_1 \leq \hat{z}_j \leq \hat{z}_{I-2}$)

Note that the computed quantities S , L , Ri , $\bar{s}$, $\bar{T}$, $\partial\sigma_T/\partial T$, $\partial\sigma_T/\partial s$, K_e , and K_m are understood to have the coordinates $(\hat{z}_j, t)$.

$$S = \left\{ \left(\frac{u(z_{j+1}) - u(z_j)}{\Delta z_j} \right)^2 + \left(\frac{v(z_{j+1}) - v(z_j)}{\Delta z_j} \right)^2 \right\}^{\frac{1}{2}} \quad (77)$$

$$\bar{s} = \frac{s(z_{j+1}) + s(z_j)}{2} \quad (78)$$

$$\bar{T} = \frac{T(z_{j+1}) + T(z_j)}{2} \quad (79)$$

Compute

$$\begin{aligned} \frac{\partial\sigma_T}{\partial T} &= .05819402 - 2(.00811465413) \bar{T} \\ &+ 3(.476600414 \times 10^{-4}) \bar{T}^2 + 2(.389187483 \times 10^{-4}) \bar{T} \bar{s} \\ &- .25310441 \times 10^{-2} \bar{s} + .28797153 \times 10^{-5} \bar{s}^2; \end{aligned} \quad (80)$$

$$\begin{aligned} \frac{\partial\sigma_T}{\partial s} &= .79701864 - .25310441 \times 10^{-2} \bar{T} \\ &+ 2(.131710842 \times 10^{-3}) \bar{s} + .389187483 \times 10^{-4} \bar{T}^2 \\ &+ 2(.287971530 \times 10^{-5}) \bar{s} \bar{T} - 3(.611831499 \times 10^{-7}) \bar{s}^2; \end{aligned} \quad (81)$$

$$L = -10^{-3} \left\{ \frac{\partial\sigma_T}{\partial T} \left(\frac{T(z_{j+1}) - T(z_j)}{\Delta z_j} \right) + \frac{\partial\sigma_T}{\partial s} \left(\frac{s(z_{j+1}) - s(z_j)}{\Delta z_j} \right) \right\}; \quad (82)$$

and

$$Ri = \frac{g \cdot L}{\rho_w [S + S_w(\hat{z}_j)]^2} \quad (83)$$

If $(S + S_w)^2 = 0$, check L ; if $L < 0$, go to A.6.2.3; if $L = 0$, set $Ri = 0$; and if $L > 0$, set $Ri = Ri_{\max}$ ($Ri_{\max} = 10^{16}$). If $Ri \geq 0$, proceed as in A.6.2.1; if $-0.048 < Ri < 0$, proceed as in A.6.2.2; if $Ri < -0.048$, proceed as in A.6.2.3.

A.6.2.1 If $Ri \geq 0$

$$K_m = K_0(\hat{z}_j)[S + S_w(\hat{z}_j)][1 + \beta_v Ri]^{-n_v} \quad (84a)$$

$$K_e = K_0(\hat{z}_j)[S + S_w(\hat{z}_j)][1 + \beta_T Ri]^{-n_T} \quad (84b)$$

and proceed to Section A.7.

A.6.2.2 If $-0.048 < Ri < 0$

$$K_m = K_0(\hat{z}_j)[S + S_w(\hat{z}_j)][1 - \alpha Ri]^{-2} \quad (85a)$$

$$K_e = \frac{K_m}{1 - \alpha Ri} \quad (85b)$$

and proceed to Section A.7.

A.6.2.3 If $Ri \leq -0.048$

$$K_e = \frac{h}{k_1^2} \left(\hat{z}_j + \frac{\lambda \delta}{2} \right)^2 \cdot \left| \frac{g \cdot L}{\rho_w} \right|^{\frac{1}{2}} \quad (86a)$$

$$\begin{aligned} K_m &= K_e \left(\frac{3}{C} \right)^{-1/2} \cdot |Ri|^{-1/6} ; & (S + S_w)^2 > 0 , \\ &= 0 ; & (S + S_w)^2 = 0 . \end{aligned} \quad (86b)$$

A.6.3 The Soil Layer

When the subsurface is soil, a soil conductivity coefficient is prescribed, K_T , and used in making soil temperature predictions.

A.7 Infrared and Solar Radiation Computations

Program specifications for the computation of infrared and solar radiation will be given in a forthcoming report to be written by Dr. Marshall A. Atwater at the Center for the Environment and Man, Inc. under IFYGL sponsorship.

A.8 Solar Absorption in the Ocean

Solar radiation absorbed by the ocean, I_0 , is dependent on the incident solar radiation at the interface, $I(z_{I+})$, and the surface albedo. Therefore, the amount of energy available for heating the ocean is given by

$$I_0 = I(z_{I+})(1 - a) \quad (87)$$

where a is the albedo computed from

$$a = - .0139 + .0467 \tan Z \quad (88)$$

with a minimum value of .03. This equation is based on results of Sverdrup, et al. (1942).

The transmission at any level z is given by

$$I_z = I_0 \exp(-\kappa_w |z| \sec Z) , \quad (89)$$

where κ_w is obtained by linear interpolation using Table 1 (Section 2.2.4.2).

The radiation absorbed in each water grid layer is calculated from the difference in radiative flux between the top and the bottom of the water layer. In the uppermost layer,

$$R_H = I_0 - I_{I-1} \quad (90)$$

and the layer B+1 (the bottom layer)

$$\Delta I_{B+1} = I_{B+1} - 0 = I_{B+1} \quad (91)$$

In the remaining layers, ΔI is computed similarly from

$$\Delta I_i = I_{i-1} - I_i \quad (92)$$

The heating rate at level i ($i = B+1, \dots, I_-$) is computed from

$$\left(\frac{dT}{dt} \right)_i = \frac{\rho_w}{c_w} \frac{\Delta I_i}{\Delta z_{i-1}} \quad (93)$$

where heating is applied to the midpoint of the layer.

A.9 Geostrophic Wind (Current) at Each Level at Each Time Step

In the following two sections (A.9.1 and A.9.2), $U_g(z_N, t)$, $V_g(z_N, t)$, $U_g(z_{I_-}, t)$, and $V_g(z_{I_-}, t)$ are computed by linear interpolation from the values of $U_g(z_N, t_1)$, $V_g(z_N, t_1)$, $U_g(z_{I_-}, t_1)$, and $V_g(z_{I_-}, t_1)$ at input times t_1 for the RIGID LID version of the model. The values of $U_g(z_{I_-}, t)$ and $V_g(z_{I_-}, t)$ are computed from the slope of the water surface in the FREE SURFACE version for a land subsurface, $U_g(z_{I_-}, t)$ and $V_g(z_{I_-}, t)$ are zero.

A.9.1 The Atmospheric Layer ($j = I+1, \dots, N-1$)

$$U_g(z_j, t) = \frac{U_g(z_N, t) \cdot T(z_j, t)}{T(z_N)} + \frac{g \cdot T(z_j, t)}{f} \left\{ \sum_{i=j+1}^N \frac{1}{2} \left(\frac{\Delta z_i}{T^2(z_i)} \right. \right. \\ \left. \left. \cdot \frac{\partial T}{\partial y}(z_i) + \frac{\Delta z_{i-1}}{T^2(z_{i-1})} \cdot \frac{\partial T}{\partial y}(z_{i-1}) \right) \right\} \quad (94a)$$

and

$$V_g(z_j, t) = \frac{V_g(z_N, t) \cdot T(z_j, t)}{T(z_N)} - \frac{g \cdot T(z_j, t)}{f} \left\{ \sum_{i=j+1}^N \frac{1}{2} \left(\frac{\Delta z_i}{T^2(z_i)} \right. \right. \\ \left. \left. \cdot \frac{\partial T}{\partial x}(z_i) + \frac{\Delta z_{i-1}}{T^2(z_{i-1})} \cdot \frac{\partial T}{\partial x}(z_{i-1}) \right) \right\} \quad (94b)$$

where

$$\frac{\partial T}{\partial y}(z_j) = \frac{\partial T}{\partial y_0}(z_j) - \frac{\partial T}{\partial z}(z_j) \frac{\partial \xi}{\partial y} \quad (95a)$$

$$\frac{\partial T}{\partial x}(z_j) = \frac{\partial T}{\partial x_0}(z_j) - \frac{\partial T}{\partial z}(z_j) \frac{\partial \xi}{\partial x} \quad (95b)$$

Since vertical grid points are most often unequally spaced and the vertical temperature gradient is approximated by the following weighted center difference,

$$\frac{\partial T}{\partial z}(z_j) = \left(\frac{\Delta z_j}{\Delta z_j + \Delta z_{j+1}} \right) \left(\frac{T(z_{j+1}) - T(z_j)}{\Delta z_{j+1}} \right) + \left(\frac{\Delta z_{j+1}}{\Delta z_j + \Delta z_{j+1}} \right) \left(\frac{T(z_j) - T(z_{j-1})}{\Delta z_j} \right) \quad (95c)$$

The horizontal gradients of the temperature relative to terrain are space centered gradients and are calculated from formulas presented in Section A.13.2.

A.9.2 The Water Subsurface ($j = 1, \dots, I-1$)

$$\frac{\partial \rho}{\partial y}(\hat{z}_j, t) = 10^{-3} \left[\frac{\partial \sigma_T}{\partial T}(\hat{z}_j, t) \frac{\partial \bar{T}_w}{\partial y}(\hat{z}_j) + \frac{\partial \sigma_T}{\partial s}(\hat{z}_j, t) \frac{\partial \bar{s}}{\partial y}(\hat{z}_j) \right], \quad (96a)$$

$$\frac{\partial \rho}{\partial x}(\hat{z}_j, t) = 10^{-3} \left(\frac{\partial \sigma_T}{\partial T_w}(\hat{z}_j, t) \frac{\partial \bar{T}_w}{\partial x}(\hat{z}_j) + \frac{\partial \sigma_T}{\partial s}(\hat{z}_j, t) \frac{\partial s}{\partial x}(\hat{z}_j) \right). \quad (96b)$$

The horizontal gradients of water temperature and salinity indicated in these formulas are vertically averaged; e.g.,

$$\frac{\partial T_w}{\partial x}(\hat{z}_{j-1}) = \frac{1}{2} \left(\frac{\partial T_w}{\partial x}(z_j) + \frac{\partial T_w}{\partial x}(z_{j-1}) \right). \quad (97)$$

Using the results of eqs. (96a) and (96b), compute

$$U_g(z_j, t) = U_g(z_{I-}, t) + \frac{g}{f} \sum_{i=j}^{I-1} \frac{\Delta z_i}{\rho_w} \frac{\partial \rho}{\partial y}(\hat{z}_i, t), \quad (98a)$$

$$V_g(z_j, t) = V_g(z_{I-}, t) - \frac{g}{f} \sum_{i=j}^{I-1} \frac{\Delta z_i}{\rho_w} \frac{\partial \rho}{\partial x}(\hat{z}_i, t). \quad (98b)$$

The values of $U_g(z_{I-})$ and $V_g(z_{I-})$ in the FREE SURFACE version of the model are calculated from

$$U_g(z_{I-}, t) = -\frac{g}{f} \frac{\partial \eta}{\partial y}, \quad (99a)$$

$$V_g(z_{I-}, t) = +\frac{g}{f} \frac{\partial \eta}{\partial x}. \quad (99b)$$

For a soil subsurface, U_g and V_g are, of course, zero.

A.10 Interface Values

The boundary and interface values are computed for each station at each time step.

A.10.1 Humidity

The saturated humidity at the interface is computed from

$$q_s(z_{I-}, t) = \frac{3.7943}{1013.2} 10^{xp} \quad (100)$$

where

$$ap = \left\{ 3 + 7.5 \frac{T(z_{I+},t) - 273.16}{T(z_{I+},t) - 35.66} \right\}. \quad (101)$$

The interface humidity is computed from

$$q(z_{I+},t) = M \cdot q_s(z_{I+},t) + (1 - M) q(z_{I+1},t) \quad (102)$$

where M is input for a soil subsurface and equals 1 for a water subsurface.

A.10.2 Winds, Currents, and Salinity

Whenever $\delta \neq 0$, always a water subsurface, the computations proceed for the interface value for u , v , and the salinity as follows:

$$u(z_{I-}) = \frac{\frac{\rho_{A m}^K(\hat{z}_{I+1}) \cdot u(z_{I+1})}{\Delta z_{I+1}} + \frac{\rho_{w m}^K(\hat{z}_{I-1}) \cdot u(z_{I-1})}{\Delta z_{I-1}}}{\frac{\rho_{A m}^K(\hat{z}_{I+1})}{\Delta z_{I+1}} + \frac{\rho_{w m}^K(\hat{z}_{I-1})}{\Delta z_{I-1}}} \quad (103a)$$

$$v(z_{I-}) = \frac{\frac{\rho_{A m}^K(\hat{z}_{I+1}) \cdot v(z_{I+1})}{\Delta z_{I+1}} + \frac{\rho_{w m}^K(\hat{z}_{I-1}) \cdot v(z_{I-1})}{\Delta z_{I-1}}}{\frac{\rho_{A m}^K(\hat{z}_{I+1})}{\Delta z_{I+1}} + \frac{\rho_{w m}^K(\hat{z}_{I-1})}{\Delta z_{I-1}}} \quad (103b)$$

$$E = -10^{-3} \cdot \rho_{A e}^K(\hat{z}_{I+1}) \left(\frac{q(z_{I+1}) - q(z_{I+})}{z_{I+1}} \right) \quad (104)$$

$$F = \frac{s(z_{I-1})(E - P_r)}{1 - s(z_{I-1}) \times 10^{-3}} \quad (105)$$

$$s(z_{I-}) = -\frac{F}{\rho_{w e}^K(\hat{z}_{I-1})} \cdot \Delta z_{I-1} + s(z_{I-1}). \quad (106)$$

The values of K_e and K_m at the grid level adjacent to the interface are given by

$$K_m(\hat{z}_{I-1}) = K_e(\hat{z}_{I-1}) = K_0(\hat{z}_{I-1}) \cdot S_w(\hat{z}_{I-1}) \quad (107a)$$

$$K_m(\hat{z}_{I+1}) = K_e(\hat{z}_{I+1}) = K_0(\hat{z}_{I+1}) \cdot S_w(\hat{z}_{I+1}) \quad (107b)$$

where K_0 is computed from eq. (68) if $\lambda \neq 0$, or from eq. (69) if $\lambda = 0$ (these coefficients are a function of time for $\lambda = 0$). Then proceed with Section A.10.3.

When $\delta = 0$ and the subsurface is water, the interface values of u , v , and s are computed as follows. Compute the value

$$B_1 = \frac{1}{k} \ln \left| \frac{z_{I+1}}{\lambda} \right|, \quad (108a)$$

$$B_2 = \frac{1}{k} \ln \left| \frac{z_{I-1}}{\lambda} \right|. \quad (108b)$$

Then compute

$$S(z_{I+1}) = [u^2(z_{I+1}) + v^2(z_{I+1})]^{\frac{1}{2}}, \quad (109a)$$

$$S(z_{I-1}) = [u^2(z_{I-1}) + v^2(z_{I-1})]^{\frac{1}{2}}. \quad (109b)$$

If $\lambda < 0$, compute

$$u^* = \frac{S(z_{I+1})}{B_1} \quad (110)$$

and

$$S(z_{I+}) = S(z_{I-}) = S(z_{I-1}) + u^* B_2 \sqrt{\rho_A / \rho_w} \quad (111)$$

and proceed with computations from the computation of $u(z_I)$ below.

If $\lambda > 0$, compute

$$u^* = [S(z_{I+1}) - S(z_{I-1})][B_1 + \sqrt{\rho_A/\rho_w} \cdot B_2]^{-1}, \quad (112)$$

and

$$S(z_{I+}) = S(z_{I-}) = S(z_{I+1}) - u^* B_1. \quad (113)$$

The computation proceeds with the calculation of $u(z_I)$ and other variables as follows:

$$u(z_{I+}) = u(z_{I-}) = u(z_{I+1}) - \left(\frac{u(z_{I+1}) - u(z_{I-1})}{S(z_{I+1}) - S(z_{I-1})} \right) [S(z_{I+1}) - S(z_{I-})] \quad (114a)$$

$$v(z_{I+}) = v(z_{I-}) = v(z_{I+1}) - \left(\frac{v(z_{I+1}) - v(z_{I-1})}{S(z_{I+1}) - S(z_{I-1})} \right) [S(z_{I+1}) - S(z_{I-})] \quad (114b)$$

$$q^* = [q(z_{I+1}) - q(z_{I+})] B_1^{-1}; \quad K_m(z_{I+1}) = |u^*|^2 \frac{\Delta \hat{z}_{I+1}}{S(z_{I+1})} \quad (115)$$

$$E(z_{I+}) = -10^{-3} \cdot \rho_A \cdot |u^*| \cdot q^* - P_r; \quad K_e(\hat{z}_{I+1}) = K_m(\hat{z}_{I+1}) \quad (116)$$

$$F(z_{I-}) = s(z_{I-1}) \cdot \frac{E}{1 - s(z_{I-1}) \cdot 10^{-3}}; \quad K_m(\hat{z}_{I-1}) = |u^*|^2 \frac{\Delta \hat{z}_{I-1}}{|S(z_{I-}) - S(z_{I-1})|} \sqrt{\frac{\rho_A}{\rho_w}} \quad (117)$$

$$s^* = \frac{F}{\sqrt{\rho_A \rho_w} \cdot |u^*|}; \quad K_e(\hat{z}_{I-1}) = K_m(\hat{z}_{I-1}) \quad (118)$$

and

$$s(z_{I-}) = s(z_{I-1}) + s^* \cdot B_2. \quad (119)$$

When the subsurface is land, $\delta = 0$ and $\lambda < 0$ (i.e., $\lambda = -z_0$).

The computations follow the previous section for the water subsurface, except that

$$S(z_{I-}) = S(z_{I+}) = 0 . \quad (120)$$

All values of u and v at heights at and below the interface are zero.

This leads to the result

$$u(z_{I+}) = v(z_{I+}) = u(z_{I-}) = v(z_{I-}) = 0 . \quad (121)$$

Similarly,

$$s(z_{I-}) = 0 . \quad (122)$$

The remaining equations are unchanged.

A.10.3 Temperature

The interface temperature T_g is computed by using the heat balance equation

$$(T_g)_{t+\Delta t} = \left(\frac{1}{\epsilon \sigma} (R_H + R_a + R_x + P_T - A - S - L \cdot E) \right)_{t+\Delta t}^{1/4} \quad (123)$$

where R_a is the atmospheric radiation incident on the interface. The term R_H is defined as the net solar energy absorbed at the interface minus the amount transmitted (if any) to lower layers (viz., water subsurface).

The incoming radiation, both solar and infrared, is computed by methods which will be described by Dr. Atwater in a forthcoming report under IFYGL sponsorship.

The heat of vaporization, L , is calculated from

$$L = 597.3 - 0.57 (T_g - 273.16) = 753.0 - 0.57 T_g \quad (124)$$

for $T_g \geq 273.16$. If $T_g < 273.16$, then $L = 677.0$.

The value E is computed in Section A.10.2. The air heat flux is calculated from

$$A = H_A = -\rho_a c_a K_e (\hat{z}_{I+1}) \left(\frac{T(z_{I+}) - T(z_{I-1})}{\Delta z_{I+1}} \right) + \Gamma , \quad (125)$$

and the surface flux is calculated from

$$S = H_i = \rho_i c_i K_e (\hat{z}_{I-1}) \left(\frac{T(z_{I+}) - T(z_{I-1})}{\Delta z_{I-1}} \right) , \quad (126)$$

where the i subscripts in eq. (126) are taken as w or s according to the subsurface.

Compute the heat loss or gain to the interface from rain, P_T ,

$$P_T = \rho_w c_w P_r (T_r - T_{L+}) , \quad (127)$$

where P_r is the precipitation ratio, and T_r is the rainfall temperature assumed to equal the average wet bulb temperature near the sea surface.

All the parameters in eq. (123) have been previously defined in terms of $(T_g)_t$. Since eq. (123) is nonlinear in T_g , an iteration procedure is required at each time step. In the iterative procedure, R_H , R_a , R_x , and L will remain constant. The values of A , S , P_T , and E will be recomputed using the value of T_g from the previous iteration. Calculation of the right-hand side of eq. (123) using these quantities yields a provisional value for $[T_g(n)]_{t+\Delta t}$ for each iteration, $n = 1, 2, \dots$.

For the initial iteration, the balance temperature used for the right-hand side of eq. (123) is obtained by

$$[T_g(1)]_{t+\Delta t} = (T_g)_t . \quad (128)$$

In the special case when the initial value of $T_g(1)$ leads to a negative value for the expression in brackets in eq. (123), a new approximation, $T_g(2)$, is defined by

$$(T_g(2))_{t+\Delta t} = \frac{1}{2} (T_g)_t, \quad (129)$$

and the iteration continues.

For each iteration, the increment

$$\Delta_n = T_g(n+1) - T_g(n) \quad (130)$$

is computed. If $|\Delta_n| \leq 0.001$, the iteration is assumed to have converged.

Then we set

$$(T_g)_{t+\Delta t} = T_g(n+1) \quad (131a)$$

for $n = 1$, and

$$(T_g)_{t+\Delta t} = \frac{T_g(n+1) + T_g(n)}{2} \quad (131b)$$

for $n = 2, 3, 4, \dots$; at which point the iteration is terminated.

When $|\Delta_n| > 0.001$, an iterative procedure is used that assumes the temperature at the preceding time step or iteration to be near the final value. Thus, when the temperature used on the right of eq. (123) is too low, the computed temperature will be too high and vice versa.

This procedure compares the signs of Δ_n and Δ_{n-1} . Until the first change in sign, the temperature used on the right-hand side in eq. (123) for the following iteration is computed from

$$T_g(n+2) = T_g(n+1) + \Delta_n. \quad (132a)$$

After a change in sign has occurred, it is assumed that the new balance temperature is within the range $T_g(n)$ to $T_g(n+1)$. Signs of Δ_n and Δ_{n-1} are compared. When the signs are the same, the next balance temperature approximation is computed from

$$T_g(n+2) = T_g(n+1) + \frac{\Delta_n}{2} \quad (132b)$$

When the signs are opposite, the balance temperature approximation is computed from

$$T_g(n+2) = T_g(n) + \frac{\Delta_{n-1}}{2} \quad (132c)$$

The iteration is then incremented and eq. (123) is then solved using the latest approximation. A maximum of 25 iterations is used, although generally less than 10 are required.

In the iterations, the following equations may be used:

$$S(n+1) = S(n) \left(\frac{T_g(n+1) - T(z_{I-1})}{T_g(n) - T(z_{I-1})} \right) \quad (133a)$$

$$A(n+1) = A(n) \left(\frac{T(z_{I+1}) - T_g(n+1)}{T(z_{I+1}) - T_g(n)} \right) \quad (133b)$$

$$E(n+1) = E(n) \left(\frac{q(z_{I+1}) - q_s(n+1)}{q(z_{I+1}) - q_s(n)} \right) \quad (133c)$$

where $q_s(n+1)$ is calculated from the saturated specific humidity for $T_g(n+1)$.

At each time step after all iterations have been completed, a time sum of each of the components of the heat balance is computed from

$$X_t = \sum X \Delta t, \quad (134)$$

where X is R_H , R_a , A , S , $L \cdot E$, P_T , R_x , and σT_g^4 .

A.10.4 Air Pollutants

If pollutants are present, the value of the pollutant concentration is computed as follows.

Compute the source emission $S_1(t)$ as a function of time by linear interpolation from the input values of $S_1(t_i)$. Then the interface value for the first pollutant is computed from

$$P_1(z_{I+}, t) = \frac{S_1(t) \Delta z_{I+1} h_{11}}{\rho_a K_e(\hat{z}_{I+1})} + P_1(z_{I+1}, t). \quad (135a)$$

Similarly for the second pollutant, if present, compute

$$P_2(z_{I+}, t) = \frac{S_2(t) \Delta z_{I+1} h_{21}}{\rho_a K_e(\hat{z}_{I+1})} + P_2(z_{I+1}, t). \quad (135b)$$

A.10.5 Computation of Interface Fluxes for Printout

If $\delta \neq 0$, the computation proceeds as in Section A.10.5.1. If $\delta = 0$, the computation proceeds as in Section A.10.5.2.

A.10.5.1 If $\delta \neq 0$

$$\tau(\hat{z}_{I+1}, t) = \rho_a K_m(\hat{z}_{I+1}) \left(\frac{S(z_{I+1}) - S(z_{I+})}{\Delta z_{I+1}} \right), \quad (136)$$

$$H_A(\hat{z}_{I+1}, t) = -\rho_a c_a K_e(\hat{z}_{I+1}) \left(\frac{T(z_{I+1}) - T(z_{I+})}{\Delta z_{I+1}} + \Gamma \right), \quad (137)$$

$$H_w(\hat{z}_{I-1}, t) = \rho_w c_w K_e(\hat{z}_{I-1}) \left(\frac{T(z_{I+}) - T(z_{I-1})}{\Delta z_{I-1}} \right), \quad (138)$$

where $S(z_j)$ is computed from eq. (109a) and an analogous equation with E and F computed in Section A.10.2 for $\delta \neq 0$.

A.10.5.2 If $\delta = 0$

$$\tau(\hat{z}_{I+1}, t) = \rho_a \cdot u^*{}^2, \quad (139)$$

$$H_A(\hat{z}_{I+1}, t) = -\rho_a c_a \cdot |u^*| \cdot [T(z_{I+1}) - T(z_{I+}) + \Gamma \cdot \Delta z_{I+1}] \cdot [B_1]^{-1}, \quad (140)$$

$$H_1(\hat{z}_{I-1}, t) = \rho_1 c_1 \cdot |u^*| \cdot [T(z_{I+}) - T(z_{I-1})] [B_2]^{-1}, \quad (141)$$

where the i subscripts in eq. (141) are taken as w or s according to the subsurface. E and F are computed in Section A.10.2 for $\delta = 0$, and u^* is computed from eq. (110) or (112) for $\lambda < 0$ and $\lambda > 0$, respectively.

A.11 Upper and Lower Boundary Values

A.11.1 Winds and Currents

The winds and currents at the upper and lower levels are computed from the geostrophic winds calculated in Section A.9 or are prescribed through linear interpolation of the input values of $U_g(z_N, t_1)$ and $V_g(z_N, t_1)$. The upper level winds are given by

$$U(z_N, t) = V_g(z_N, t) \quad (142a)$$

$$V(z_N, t) = U_g(z_N, t), \quad (142b)$$

where linear interpolation with respect to time is used to obtain values of

$U_g(z_N, t)$ and $V_g(z_N, t)$ at times for which they are not specified.

In the RIGID LID version of the model, at stations with a water sub-surface, the currents are computed at the lowest grid level, z_1 , from

$$u(z_1, t+1) = u(z_1, t) + \Delta t \cdot f[v(z_1, t) - V_g(z_1, t)] \quad (143a)$$

$$v(z_1, t+1) = v(z_1, t) + \Delta t \cdot f[U_g(z_1, t) - u(z_1, t)] \quad (143b)$$

where $V_g(z_1, t)$ and $U_g(z_1, t)$ are obtained from the equations in Section A.9. The boundary conditions impose restrictions on the solutions of eqs. (143a) and (143b); viz., for a coastal corner station,

$$u(z_1, t) = 0 \quad (144)$$

$$v(z_1, t) = 0; \quad (145)$$

for a coastal station with a coast oriented in an east-west direction, eq. (144), and for a coastal station with a coast oriented in a north-south direction, eq. (145).

The FREE SURFACE version of the model sets the current velocity components at water stations equal to zero at and below the bottom boundaries, i.e.,

$$u(z_j, t) = v(z_j, t) = 0, \quad (146)$$

where $j = 1, \dots, B$.

A.11.2 Temperature, Humidity, Salinity, and Pollutants

The upper and lower boundary values (at $z = z_1, z_N$) are held constant for T, q, s, P_1 , and P_2 .

A.11.3 Printout of Boundary Fluxes

$$\tau(z_N, t) = \rho_a \cdot K_m(\hat{z}_N, t) \cdot S(\hat{z}_N, t) \quad (147)$$

$$\tau(z_1, t) = \rho_w \cdot K_m(\hat{z}_1, t) \cdot S(\hat{z}_1, t) \quad (148)$$

$$H_A(\hat{z}_N, t) = -\rho_a \cdot c_a \cdot K_e(\hat{z}_N, t) \left[\frac{T(z_N) - T(z_{N-1})}{\Delta z_N} + \Gamma \right] \quad (149)$$

$$H_1(\hat{z}_1, t) = \rho_1 \cdot c_1 \cdot K_e(\hat{z}_1, t) \left[\frac{T(z_2) - T(z_1)}{\Delta z_1} \right] \quad (150)$$

$$E(\hat{z}_N, t) = -\rho_a \cdot K_e(\hat{z}_N, t) \left[\frac{q(z_N) - q(z_{N-1})}{\Delta z_N} \right] \quad (151)$$

$$F(\hat{z}_1, t) = \rho_1 \cdot K_e(\hat{z}_1, t) \left[\frac{s(z_2) - s(z_1)}{\Delta z_1} \right] \quad (152)$$

where the 1 subscripts in eqs. (150) and (152) are taken as w or s according to the subsurface.

A.12 Solution of the Finite-Difference Equation

The following sets of equations are solved simultaneously, one station at a time, for each station in the grid through an implicit three time level differencing scheme which makes use of Gaussian elimination techniques for tri-diagonal and block tri-diagonal matrices. Therefore, there are no subscripts indicating horizontal grid locations; the subscript j denotes grid location in the vertical and superscript t designates the time level, viz., $t - 1$ = past, t = present, $t + 1$ = future. The matrix of coefficients contains two less rows than vertical grid levels in a layer (air, land, or water); this is because the values of the dependent variables are

TABLE A-1
Definitions of Generalized Coefficients

Quantity	$T_w(z_2 \leq z \leq z_{I-1})$	$T_A(z_{I+1} \leq z \leq z_{N-1})$	q	s	$P_1(z_2 \leq z \leq z_{I-1})_{I-1,2}$	$P_1(z_{I+1} \leq z \leq z_{N-1})_{I-1,2}$
$K_a(z_j)$	$K_e(z_j)$	$K_e(z_j)$	$K_e(z_j)$	$K_e(z_j)$	$K_e(z_j)$	$K_e(z_j)$
$A_a(z_j)$	$-\left[u \frac{\partial T_w}{\partial x} + v \frac{\partial T_w}{\partial y}\right]_j + \left[\left(\frac{\partial T_w}{\partial t}\right)_{sol}\right]_j$	$-\left[u \frac{\partial T_A}{\partial x} + v \frac{\partial T_A}{\partial y}\right]_j + \left[\frac{2\Gamma}{(\Delta z_j + \Delta z_{j+1})}\right] \cdot [K_e(z_j) - K_e(z_{j+1})] + \left[\left(\frac{\partial T_A}{\partial t}\right)_{1r}\right]_j + \left[\left(\frac{\partial T_A}{\partial t}\right)_{sol}\right]_j - W(z_j) \cdot r$	$-\left[u \frac{\partial q}{\partial x} + v \frac{\partial q}{\partial y}\right]_j$	$-\left[u \frac{\partial s}{\partial x} + v \frac{\partial s}{\partial y}\right]_j$	$-\left[u \frac{\partial P_1}{\partial x} + v \frac{\partial P_1}{\partial y}\right]_j - \left[u \frac{\partial P_1}{\partial x} + v \frac{\partial P_1}{\partial y}\right]_j + S_{P_1}(z_j) + S_{P_1}(z_j)$	$S_{P_1}(z_j) = \frac{2S_{1,1l}}{(z_{j+1} - z_{j-1}) \cdot \rho a}$
						$z = (I_+ - j) \leq 6 \quad z = (j - I_-) \leq 6$
						$z > 6 \quad S_{P_1}(z_j) = 0 \quad z > 6$
$x_1 = x_2$	$T_w(z_2)$	$T_A(z_{I+1})$	$q(z_{I+1})$	$s(z_2)$	$P_1(z_2)$	$P_1(z_{I+1})$
$x_j = x_{j+1}$	$T_w(z_{j+1})$	$T_A(z_{I+1+j})$	$q(z_{I+1+j})$	$s(z_{j+1})$	$P_1(z_{j+1})$	$P_1(z_{I+1+j})$
$x_n = x_{n+1}$	$T_w(z_{I-1})$	$T_A(z_{N-1})$	$q(z_{N-1})$	$s(z_{I-1})$	$P_1(z_{I-1})$	$P_1(z_{N-1})$

+ Heating or cooling due to solar radiation.

* Heating or cooling due to infrared radiation.

known at the interface and the upper and lower boundaries of the boundary layer. The relationship between the x_j 's and the x_1 's is clarified in Table A-1.

A.12.1 T, q, s, P_1 , and P_2 -

The finite difference equations for T, q, s, P_1 , and P_2 take the form

$$\begin{aligned}
 d_1 &= b_1 x_1 + c_1 x_2 \\
 d_2 &= a_2 x_1 + b_2 x_2 + c_2 x_3 \\
 &\vdots \\
 d_j &= a_j x_{j-1} + b_j x_j + c_j x_{j+1} \\
 &\vdots \\
 d_n &= a_n x_{n-1} + b_n x_n
 \end{aligned} \tag{153}$$

where the x_j 's denote the unknown values of T, q, s, P_1 , or P_2 , and the coefficients are known quantities.

Generalized coefficient formulas are

$$a_1 = 0 \tag{154}$$

$$a_j = - \frac{2\Delta t}{(\Delta z_{j+1} + \Delta z_j)} \left(\frac{K_a(\hat{z}_j)}{z_j} + 0.5 w_{j+1} \right) \tag{155}$$

where $j = 2, \dots, n$;

$$c_j = - \frac{2\Delta t}{(\Delta z_{j+1} + \Delta z_j)} \left(\frac{K_a(\hat{z}_{j+1})}{\Delta z_{j+1}} - 0.5 w_{j+1} \right) \tag{156}$$

$$c_1^* = -\frac{c_1}{b_1} ; \quad (162)$$

$$d_1^* = +\frac{d_1}{b_1} ; \quad (163)$$

$$c_j^* = \frac{c_j}{a_j c_{j-1}^* + b_j} , \quad (164)$$

where $j = 2, \dots, n-1$;

$$d_j^* = \frac{d_j - a_j d_{j-1}^*}{a_j c_{j-1}^* + b_j} , \quad (165)$$

where $j = 2, \dots, n-1$;

$$c_n = \frac{d_n - a_n d_{n-1}^*}{a_n c_{n-1}^* + b_n} ; \quad (166)$$

$$x_j = c_j^* x_{j+1} + d_j^* , \quad (167)$$

where $j = n-1, n-2, \dots, 1$.

A.12.2 u and v

The finite-difference equations for u and v take the form

$$A_j \bar{u}_{j-1} + B_j \bar{u}_j + C_j \bar{u}_{j+1} = \bar{f}_j \quad (168)$$

where the vectors are defined:

$$\bar{u}_{j+1} = \begin{Bmatrix} u(z_j, t) \\ v(z_j, t) \end{Bmatrix} ; \quad (169)$$

$$\bar{f}_j = \begin{cases} C6 \cdot u_{j+1}^t + \Delta t \left(-fV_g(j+1) - u_{j+1}^t \left(\frac{\partial u}{\partial x} \right)_{j+1} - v_{j+1}^t \left(\frac{\partial u}{\partial y} \right)_{j+1} \right) - \frac{\delta \cdot u_{j+1}^{t-1}}{2} \\ C6 \cdot v_{j+1}^t + \Delta t \left(+fU_g(j+1) - u_{j+1}^t \left(\frac{\partial v}{\partial x} \right)_{j+1} - v_{j+1}^t \left(\frac{\partial v}{\partial y} \right)_{j+1} \right) - \frac{\delta \cdot v_{j+1}^{t-1}}{2} \end{cases} \quad (170)$$

where $j = 2, \dots, n-1$ for eqs. (169) and (170);

(171)

$$\bar{f}_1 = \begin{cases} C6 \cdot u_2^t - \Delta t \cdot fV_g(2) - \frac{\delta \cdot u_2^{t-1}}{2} + \frac{K(\hat{z}_1)}{\Delta z_1} \frac{u_1^t \cdot 2\Delta t}{\Delta z_2 + \Delta z_1} - \Delta t \left(u_2^t \left(\frac{\partial u}{\partial x} \right)_2 + v_2^t \left(\frac{\partial u}{\partial y} \right)_2 \right) \\ C6 \cdot v_2^t + \Delta t \cdot fU_g(2) - \frac{\delta \cdot v_2^{t-1}}{2} + \frac{K(\hat{z}_1)}{\Delta z_1} \frac{v_1^t \cdot 2\Delta t}{\Delta z_2 + \Delta z_1} - \Delta t \left(v_2^t \left(\frac{\partial v}{\partial x} \right)_2 + v_2^t \left(\frac{\partial v}{\partial y} \right)_2 \right) \end{cases}$$

$$f_n = \begin{cases} C6 \cdot u_{n+1}^t - \Delta t \cdot fV_g(n+1) - \frac{\delta \cdot u_{n+1}^{t-1}}{2} + \frac{K(\hat{z}_{n+1})}{\Delta z_{n+1}} \frac{u_{n+2}^t \cdot 2\Delta t}{\Delta z_n + \Delta z_{n+1}} \\ C6 \cdot v_{n+1}^t + \Delta t \cdot fU_g(n+1) - \frac{\delta \cdot v_{n+1}^{t-1}}{2} + \frac{K(\hat{z}_{n+1})}{\Delta z_{n+1}} \frac{v_{n+2}^t \cdot 2\Delta t}{\Delta z_n + \Delta z_{n+1}} \end{cases} \quad (172)$$

$$= w_{n+1} \frac{\Delta t}{\Delta z_n + \Delta z_{n+1}} \begin{pmatrix} u_{n+2}^t \\ v_{n+2}^t \end{pmatrix};$$

and the matrix elements

$$a_1 = 0; \quad (173)$$

$$a_j = - \frac{2\Delta t}{\Delta z_j + \Delta z_{j+1}} \left(\frac{K(\hat{z}_j)}{\Delta z_{j+1}} + 0.5 w_{j+1} \right) \quad (174)$$

where $j = 2, \dots, n$;

$$BR_j = C5 + \frac{2\Delta t}{\Delta z_j + \Delta z_{j+1}} \left(\frac{K(\hat{z}_j)}{\Delta z_{j+1}} + \frac{K(\hat{z}_{j+1})}{\Delta z_{j+1}} \right), \quad (175)$$

$$BG_j = -f \cdot \Delta t, \quad (176)$$

where $j = 1, \dots, n$ for eqs. (175) and (176);

$$c_1 = -\frac{2\Delta t}{\Delta z_1 + \Delta z_2} \cdot \frac{K(\hat{z}_2)}{\Delta z_2}; \quad (177)$$

$$c_j = -\frac{2\Delta t}{\Delta z_j + \Delta z_{j-1}} \left(\frac{K(\hat{z}_{j+1})}{\Delta z_{j+1}} - 0.5 w_{j+1} \right), \quad (178)$$

where $j = 2, \dots, n-1$; and

$$c_n = 0. \quad (179)$$

Terms A_j and C_j are diagonal matrices where

$$A_j = \begin{pmatrix} a_j & 0 \\ 0 & a_j \end{pmatrix} \quad (180a)$$

$$C_j = \begin{pmatrix} c_j & 0 \\ 0 & c_j \end{pmatrix} \quad (180b)$$

and B_j has the form

$$B_j = R1_j \begin{pmatrix} BR_j/R2_j & -BG_j/R2_j \\ -BG_j/R2_j & BR_j/R2_j \end{pmatrix}, \quad (180c)$$

with

$$R1_j = BR_j^2 + BG_j^2 \quad (181a)$$

and

$$R2_j = BR_j^2 - BG_j^2. \quad (181b)$$

The constants $C5$, $C6$, and δ are defined as before. Quantities for the upper and lower atmospheric and oceanic sublayers are given in Table A-2 below.

TABLE A-2
Identification of Quantities

Quantity	$u, v(z_{I+1} \leq z \leq z_{N-1})$	$u, v(z_2 \leq z \leq z_{I-1})$
K	K_m	K_m
$\bar{u}_2$	$\bar{u}_{I+1}$	$\bar{u}_2$
$\bar{u}_n$	$\bar{u}_{N-1}$	$\bar{u}_{I-1}$

Recursion formulas for the solutions of the finite-difference equations are:

$$E_1 = -B_1^{-1} C_1 ; \quad (182)$$

$$\bar{f}_1^* = B_1^{-1} \bar{f}_1 ; \quad (183)$$

$$E_j = -(A_j E_{j-1} + B_j)^{-1} C_j , \quad (184)$$

where $j = 2, \dots, n-1$;

$$\bar{f}_j^* = (A_j E_{j-1} + B_j)^{-1} (\bar{f}_j - A_j \bar{f}_{j-1}^*) , \quad (185)$$

$$\bar{u}_n = \bar{f}_n^* ; \quad (186)$$

$$\bar{u}_j = E_j \bar{u}_{j+1} + \bar{f}_j^* , \quad (187)$$

where $j = n-1, n-2, \dots, 1$. The solutions to the water velocities are subject to the boundary conditions stated in Section 2.2.4.2 of the text.

A.13 Horizontal Advection

The horizontal array of grid points is to consist of a rectangular array of equally spaced grid points with no limitation within the formulation of the FORTRAN Program on the number of stations in the grid. The horizontal gradients for each of the unknown variables, u, v, T, q, s, P_1 , and P_2 are computed according to the scheme outlined in the model formulation of Gerrity (1967).

In the FREE SURFACE version of the model, the horizontal gradients of the dependent variables are calculated every time step, but in the RIGID LID version, the number of basic time steps to elapse before recomputation of the horizontal gradients is calculated in the following way. The entire three-dimensional array is to be scanned for the maximum absolute velocity component value, c_m . The number of basic time steps to elapse is then

$$N_u = \frac{\Delta}{(\sqrt{2} + .01) |c_m| \cdot \Delta t} \quad (188)$$

A.13.1 Horizontal Advection Gradients

The horizontal gradients of a variable X_l in the x ($l = 1$) and y ($l = 2$) directions are computed for station j, k at each vertical grid level n using the form $(\delta_l X_l / \Delta x_l)_{j,k}^n$ where $(\delta_l X_l)_{j,k}^n$ is computed by

$$(\delta_1 X_1)_{j,k}^n = \begin{cases} (X_1)_{j,k}^n - (X_1)_{j-1,k}^n & \text{for } u_{j,k}^n > 0 \\ (X_1)_{j+1,k}^n - (X_1)_{j,k}^n & \text{for } u_{j,k}^n \leq 0 \end{cases}, \quad (189a)$$

$$(\delta_2 X_1)_{j,k}^n = \begin{cases} (X_1)_{j,k}^n - (X_1)_{j,k-1}^n & \text{for } v_{j,k}^n > 0 \\ (X_1)_{j,k+1}^n - (X_1)_{j,k}^n & \text{for } v_{j,k}^n \leq 0 \end{cases}. \quad (189b)$$

Whenever one of the grid points to be used in the computations above (e.g., $(X_1)_{j,0}^n$) falls outside of the horizontal array, the horizontal gradients cannot be computed and are, therefore, prescribed through input to the program (see Section A.4). These one-sided horizontal gradients are used in the advection terms, particularly in Section A.12.

A.13.2 Space-Centered Gradients

Space-centered gradients are computed from $(\delta_2 X_1 / 2\Delta x_1)_{j,k}^n$ where

$$(\delta_1 X_1)_{j,k}^n = (X_1)_{j+1,k}^n - (X_1)_{j-1,k}^n \quad (190a)$$

and

$$(\delta_2 X_1)_{j,k}^n = (X_1)_{j,k+1}^n - (X_1)_{j,k-1}^n \quad (190b)$$

for all internal points. At boundary points where u and/or v are directed into the grid, the respective space-centered gradients are not calculated but are prescribed through the model input gradients. If, on the other hand, the predicted u and/or v components at boundary points are directed out of the grid, the space-centered gradients are taken equal to the one-sided horizontal advection gradients which are calculated by the formulas in Section A.13.1.

In the FREE SURFACE version, space-centered gradients are used to calculate the terms $\partial\eta/\partial x$ and $\partial\eta/\partial y$ appearing in the equations used to compute the geostrophic currents, viz., eqs. (99a) and (99b). The finite-difference forms of these derivatives are $(\delta_x \eta / 2\Delta x)_j$, where

$$(\delta_1 \eta)_{j,k} = (\eta)_{j+1,k} - (\eta)_{j-1,k} \quad (191a)$$

and

$$(\delta_2 \eta)_{j,k} = (\eta)_{j,k+1} - (\eta)_{j,k-1} \quad (191b)$$

The value of η at the land stations is taken as zero. If the above differences are taken at open water boundaries, η is specified outside the grid.

A.13.3 The Terrain Relative Vertical Velocity

The vertical velocity relative to the terrain is prescribed or computed at each vertical grid point. In the RIGID LID version, computations are performed as follows:

- water layer

$$w(z_j) = \sum_{k=j}^{k=I-1} \frac{1}{2} \left(\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right)_{k+1} + \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right)_k \right) \Delta z_k \quad (192a)$$

where $B \leq j \leq I-1$, and $w(z_B) = 0$.

- air layer

$$w(z_j) = - \sum_{k=I_+}^{k=J-1} \frac{1}{2} \left(\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right)_{k+1} + \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right)_k \right) \Delta z_{k+1}, \quad (192b)$$

where $I_+ \leq j \leq N$, and at the interface

$$w(z_{I_-}) = w(z_{I_+}) = 0 \quad (193)$$

The FREE SURFACE version uses the equations as follows:

- water layer

$$w(z_j) = - \sum_{k=B}^{j-1} \frac{1}{2} \left(\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right)_{k+1} + \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right)_k \right) \Delta z_k, \quad (194a)$$

where $B \leq j \leq I$, and $w(z_B) = 0$.

- air layer

$$w(z_j) = w(z_{I_+}) - \sum_{k=I_+}^{j-1} \frac{1}{2} \left(\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right)_{k+1} + \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right)_k \right) \Delta z_{k+1} \quad (194b)$$

where $I_+ \leq j \leq N$, and at the interface

$$w(z_{I_-}) = w(z_{I_+}) = 0. \quad (195)$$

The water surface elevation at time t , η^t , is given by

$$\eta^t = \eta^{t-1} + w(z_{I_-}) \Delta t. \quad (196)$$

The vertical velocities and water surface elevations are computed whenever the horizontal advection gradients are calculated, i.e. every time step in the FREE SURFACE version and every N_u time step in the RIGID LID version.

A.14 Output

The output will be written on a tape or disk for later use. These records will show the height and time variations of the following parameters:

- K_e eddy diffusivity (cm^2/sec).
- P_1 pollutant 1 ($\mu\text{g}/\text{m}^3$) if present.
- P_2 pollutant 2 ($\mu\text{g}/\text{m}^3$) if present.
- q humidity (g/kg), $z_j \geq z_{I_+}$.

Ri	Richardson number.
s	salinity (g/kg), $z_j \leq z_{L-}$.
T	temperature ($^{\circ}$ K).
u	eastward wind/current component (cm/sec).
v	northward wind/current component (cm/sec).
V	wind/current speed (cm/sec).
w	vertical velocity relative to the terrain (cm/sec).
$(\partial T/\partial t)_{ir}$	infrared and solar heating rates ($^{\circ}$ K/day).

The following parameters will also be printed out. They will all be in one 600-word record for each station:

a	albedo (n.d.).
h	height of wave (cm).
M	moisture parameter (n.d.).
R_x	artificial heat source (ly/sec).
δ	steepness of characteristic wave (n.d.).
λ	wavelength of turbulent wave (cm) if water, if negative, indicates land and is $-z_0$, the roughness height (cm).
ρ	soil/water density (cal/g/ $^{\circ}$ K).
$I_v(N)$	upward solar flux at z_N (mly/sec).
$R_d(N)$	downward infrared flux at $z = z_N$ (mly/sec).
$R_u(N)$	upward infrared flux at $z = z_N$ (mly/sec).
$R_s(N)$	downward solar flux at $z = z_N$ (mly/sec).
$R_d(0)$	downward infrared flux at surface (mly/sec).
$R_u(0)$	upward infrared flux at surface (mly/sec).
$R_s(0)$	downward solar flux at surface (mly/sec).
$E(0,t)$	eddy water-vapor flux into the atmosphere at the interface g/cm ² /sec).

$F(0,t)$	eddy salinity flux into the ocean at the interface (g/cm ² /sec).
$H_A(0,t)$	eddy heat flux into the atmosphere at the interface (cal/cm ² /sec).
$H_s(0,t)$	eddy heat flux into the ocean at the interface (cal/cm ² /sec).
$\tau(0,t)$	stress at the interface (dynes/cm ²).
$E(z_N,t)$	eddy flux of latent heat at the upper boundary.
$F(z_1,t)$	eddy flux of salinity at the lower boundary.
$H_A(z_N,t)$	eddy flux of heat at the upper boundary.
$H_s(z_1,t)$	eddy flux of heat at the lower boundary.
$\tau(z_N,t)$	stress at the upper boundary.
$\tau(z_1,t)$	stress at the lower boundary.

The following time sums will be printed and stored on tape (units = ly).

$A(t)$	heat flux into the atmosphere.
$b(t)$	outgoing infrared flux at surface.
$[L \cdot E](t)$	latent heat flux.
$P(t)$	heat flux due to precipitation.
$R_a(t)$	incoming infrared flux at surface.
$R_{se}(t)$	solar flux used for heating interface.
$R_x(t)$	artificial heat source.
$S(t)$	heat flux into the subsurface.

Additional printed variables for the FREE SURFACE version include:

$\eta(x,y,t)$	departure of the water surface from a mean state (cm).
$\frac{\partial \eta}{\partial x}(x,y,t)$	slope of the water surface in the x-direction (n.d.).
$\frac{\partial \eta}{\partial y}(x,y,t)$	slope of the water surface in the y-direction (n.d.).

Appendix B

A Terrain-Based Coordinate System

The choice of a terrain relative vertical coordinate axis allows for a convenient incorporation of topographic effects in the solutions of the equations of motion. An additional property of this coordinate system is its compatability with surface data observation networks, since station observations are obtained in constant z surfaces, while horizontal mesh distances are given in constant x surfaces (see Page 8 of the text for a definition of x and z).

The horizontal derivative of the dependent variable X , most readily obtained from observations, may be defined (see Fig. B) as

$$\frac{\partial X}{\partial x_0} = \lim_{\Delta x \rightarrow 0} \left(\frac{X_2 - X_0}{\Delta x} \right) , \quad (197)$$

where z is fixed. The relevant horizontal derivative in the coordinate system relative to an absolute reference surface may be defined as

$$\frac{\partial X}{\partial x} = \lim_{\Delta x \rightarrow 0} \left(\frac{X_1 - X_0}{\Delta x} \right) , \quad (198)$$

where z is fixed. Equations (197) and (198) together may be written

$$\frac{\partial X}{\partial x} = \lim_{\Delta x \rightarrow 0} \left(\frac{X_2 - X_0}{\Delta x} - \frac{X_1 - X_2}{\Delta x} \frac{\Delta \xi}{\Delta z} \right) . \quad (199)$$

Taking limits sequentially and using the definition given in eq. (197),

$$\frac{\partial X}{\partial x} = \frac{\partial X}{\partial x_0} - \frac{\partial x}{\partial z} \frac{\partial \xi}{\partial x} , \quad (200)$$

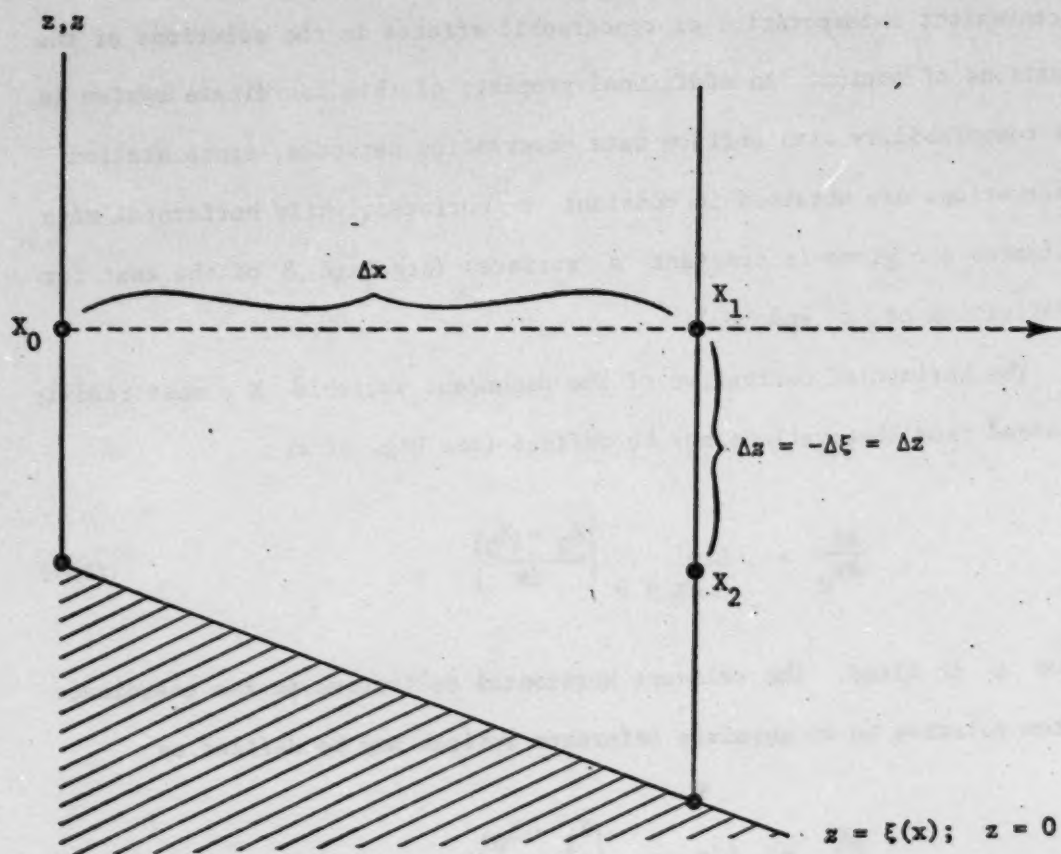


Figure B. Schematic diagram illustrating the relationship between the gradient in a surface parallel to the terrain (z constant), and the gradient in a horizontal surface (z constant).

and similarly,

$$\frac{\partial X}{\partial y} = \frac{\partial X}{\partial y_0} - \frac{\partial X}{\partial z} \frac{\partial \xi}{\partial y} . \quad (201)$$

These horizontal derivatives could have been derived through an application of the chain rule, viz.,

$$X = X(x, y, z(x, y, z)) \quad (202)$$

and

$$z = z - \xi . \quad (203)$$

Therefore,

$$\left. \frac{\partial X}{\partial x} \right|_{z \text{ constant}} = \left. \frac{\partial X}{\partial x} \right|_{z \text{ constant}} + \frac{\partial X}{\partial z} \frac{\partial z}{\partial x} = \left. \frac{\partial X}{\partial x} \right|_{z \text{ constant}} - \frac{\partial X}{\partial z} \frac{\partial \xi}{\partial x} . \quad (204)$$

Appendix C

Atmospheric Radiation Computations for an Urban Meteorological Pollutant Model

M. Atwater

C.1 INTRODUCTION

The purpose of these specifications is to define, in detail, the radiative computations used in a generalized three-dimensional model of the atmosphere and land or water subsurface. Section C.2 will list the symbols, general definitions and assumptions used in the radiation model. Symbols may vary slightly from the symbols used in other specifications given previously. Section C.3 will describe the infrared computation and Section C.4 will describe the solar radiation computations. Section C.5 will include the effects of terrain on both solar and infrared computations. However, it should be noted that the terrain effects have not been included in the results of the final report. Their effects will be tested in the future.

The vertical profiles of pressure, temperature, and humidity to level N (level H in previous specifications) are obtained from the values at each time step for each horizontal grid point. Input values of pressure, temperature, and humidity are specified for all levels above level N and are constant over the entire grid. Aerosols are also specified above level N. Aerosols can be specified to be the first pollutant below level N and would be computed within the model. This was not done during the present contract period. clouds are input at any level, above or below level N, and are linearly interpolated in time over input values.

C.2 GENERAL DEFINITIONS AND ASSUMPTIONS

C.2.1 Vertical Grid and Symbols

The radiation computations described here use a vertical grid shown in Figure C at each horizontal grid point. There are n_g levels from the surface to the top of the atmosphere, and there are N ($1 \leq N < n_g$) levels where the net infrared and solar fluxes are computed. If $N \geq 3$, radiative heating rates are computed for all levels from level 2 to $N - 1$.

The symbols will be separated into two types. First are symbols that have well defined meaning in relation to the radiation model. The second type are symbols used only once or twice, and often without any specific physical meaning. They are mainly used to make the equations more easily read or for ease of programming.

C.2.1.1 Radiation and Model Variables

a	surface albedo (n.d.).
B_a	aerosol absorption coefficient (cm^{-1}).
B_s	aerosol scattering coefficient (cm^{-1}).
c_p	specific heat of air (.24 cal/gm/°K).
c_v	incoming solar flux on horizontal surface at top of atmosphere (n.d.).
$F_n(z)$	net flux at level n (ly/sec).
g	gravitational acceleration (= 980 cm/sec ²).
h	local hour angle (deg).
I_0	solar constant (= 1.95 ly/min).
M	solar optical path length (n.d.).
n_c	number of cloud layers.
p	pressure (mb).
P	concentration of aerosols ($\mu\text{gm}/\text{m}^3$).

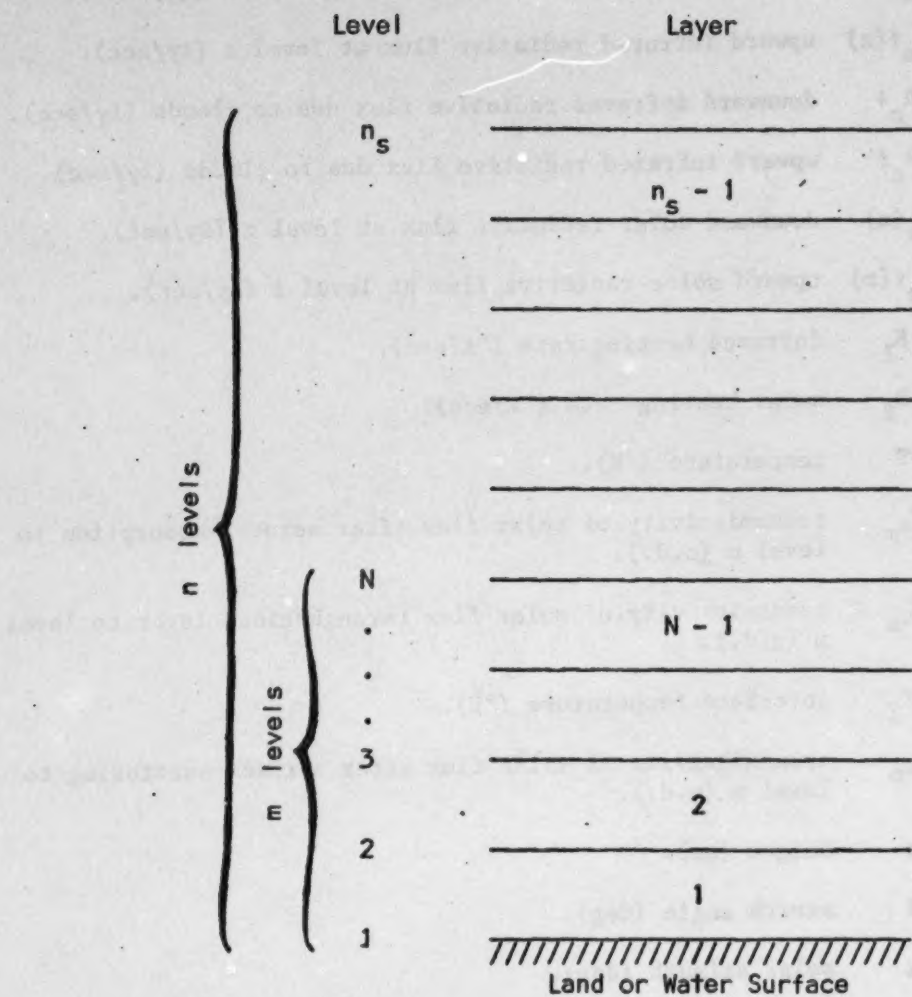


Figure C. Vertical grid for atmospheric radiation computation.

q	specific humidity (gm/kgm).
R	gas constant for dry air (2.87×10^6 erg/ g/°K).
$R_a^-(z)$	downward infrared radiative flux at level z (ly/sec).
$R_a^+(z)$	upward infrared radiative flux at level z (ly/sec).
R_c^-	downward infrared radiative flux due to clouds (ly/sec).
R_c^+	upward infrared radiative flux due to clouds (ly/sec).
$R_s^-(z)$	downward solar radiative flux at level z (ly/sec).
$R_s^+(z)$	upward solar radiative flux at level z (ly/sec).
S_1	infrared heating rate (°K/sec).
S_2	solar heating rate (°K/sec).
T	temperature (°K).
T_{am}	transmissivity of solar flux after aerosol absorption to level m (n.d.).
T_{cm}	transmissivity of solar flux through cloud layer to level m (n.d.).
T_I	interface temperature (°K).
T_{sm}	transmissivity of solar flux after aerosol scattering to level m (n.d.).
z	height (km).
Z	zenith angle (deg).
α	solar azimuth (deg).
α_p	conversion factor for assumed aerosol size distribution for use with aerosol radiation coefficients ($m^3/\mu gm$).
β	angle between terrain slope and horizontal (deg).
δ	declination (deg).
$\Delta F_n(z_n)$	solar flux absorbed in layer above level z (ly/sec).
Δu_a	path length increment for aerosol (cm).
Δu_c	path length increment for carbon-dioxide (cm).
Δu_w	path length increment for water vapor (cm).

ϵ	emissivity due to water vapor (n.d.).
ϵ_l	fractional cloud amount for cloud layer l (n.d.).
η	azimuth of terrain slope (deg).
κ	infrared absorption coefficient for aerosol (cm^{-1}).
σ	Stefan-Boltzmann constant ($1.354 \times 10^{-12} \text{ ly}/^\circ\text{K}^4/\text{sec}$).
τ_c	transmissivity due to carbon dioxide (n.d.).
$\tau_{n,m}$	transmission between levels n and m (n.d.).
$\tau(n,m)$	value in transmissivity matrix (n.d.).
ϕ	latitude (deg).
ψ	transmissivity of solar flux through a cloud of given type with a given path length (n.d.).
$\frac{\partial H}{\partial x}$	gradients of terrain H (n.d.).
$\frac{\partial H}{\partial x}$	
$\frac{\partial T}{\partial t}$	radiative heating rate for layer ($^\circ\text{K}/\text{sec}$).

C.2.1.2 Temporary Symbols

The following symbols have little, if any, significant meaning other than to make the equations more readable and easier to program. Therefore, only the variables will be given and the equations that define the variables.

<u>Variable</u>	<u>Equation Defined</u>	
A_m	11(+4) *	* Where eq. 11(+4) is the fourth equation after equation (11). This procedure in identifying equations follows throughout Appendix C.
E	15	
F_m	11(+10)	
G	11(+8)	
R_+	1d, 4(+1)	
R_a^+	6d, 8	
R_s^+	14	
T_1	11(+6)	
T_2	11(+7), 12(+3)	

<u>Variable</u>	<u>Equation Defined</u>
T_a	13
u_a	7(+2), 11(+1)
u_n	1(-3)
u_{cn}	1(-3)
V	10(+3)
W	11(+9)
Y	11(+5)
ϵ_a	5, 3, 6c, 8, 1c
ϵ_c	1b, 3(+1), 7(+1), 6b

C.2.2 General Assumptions

The radiation model described here is designed for use within the boundary layer of the atmosphere. Its applicability is probably valid within the troposphere.

The radiative fluxes, both upward and downward solar and infrared, are computed at each time step. Both solar and infrared use empirical equations to cover their respective parts of the spectrum. In addition to standard absorbers and scatterers, clouds and pollutant or natural aerosols are included in the model. Using appropriate radiation coefficients, a pollutant gas can be added to, or substituted for, the aerosols. The influence of clouds is estimated using the following assumptions.

- 1) The amount of coverage of two or more layers is equal to the product of the individual coverage. This is equivalent to assuming a horizontally uniform distribution of clouds.
- 2) The thickness of the clouds below level N is assumed to be one layer.
- 3) The clouds are black for atmospheric radiation.

The method used here follows that outlined by Manabe and Strickler (1964).

C.2.3 Optical Path Lengths

Increments of the optical path length for each of the absorbers and scatterers are computed for $n_g - 1$ layers of the atmosphere.

The path length increments for water vapor are computed for

$$\Delta u_{w1} = \frac{(p_1 - p_{i+1})(q_1 + q_{i+1})}{2g}$$

The path length increment for carbon dioxide is

$$\Delta u_{c1} = .4148239 (p_1 - p_{i+1}) ,$$

which assumes 320 ppm for the atmospheric carbon dioxide.

The path length increment for aerosols is computed from

$$\Delta u_{a1} = \frac{\alpha_p}{2} [(P)_1 + (P)_{i+1}](z_{i+1} - z_1) \times 10^{-5}$$

where P is the aerosol concentration. Above level N , the layer thickness needs to be computed. This is done by using the hydrostatic equation, which results in

$$z_{i+1} - z_1 = \frac{R}{g} \frac{T_1}{P_1} (p_1 - p_{i+1})$$

In all cases, the path length increments are computed from the surface $i = 1$ to the top layer of the atmosphere, i.e. $i = n_g - 1$. The layer thickness is only needed for $i \geq N$.

C.3 INFRARED RADIATION

C.3.1 Transmissivity Matrix

A transmissivity matrix for dimension N by $n_g - 1$ is computed at certain specified intervals, currently six hours, to reduce the computer time. The indices used with the transmissivity matrix will be m with a range of 1 to N and n with a range of 1 to $n_g - 1$.

For each level from 1 to N , downward and upward infrared radiation will be computed. As the transmission is a function of the total path length from the level m to a given layer n , the path length is computed first, and then the transmission is computed. The total path length for water vapor u is computed from

$$u_n = \sum_{i=m}^{n-1} \Delta u_{w1}, \quad n \geq m ;$$

$$u_n = \sum_{i=m}^{m-1} \Delta u_{w1}, \quad n < m .$$

Identical equations except for the replacement of Δu_w with Δu_c are used for the total path lengths for carbon dioxide. From the total path length, the transmission (or emissivity) is computed. The transmissivity (or emissivity) is computed from equations given in Table C-1 for water vapor and carbon dioxide.

Then each value of the transmissivity matrix is computed from

$$\tau(n,m) = .815 - \epsilon + \tau_c .$$

The above procedure is repeated for all valid values of m and n except $m = n$. The matrix $\tau(n,m)$ is used for later computations.

TABLE C-1
Infrared Diffuse Transmission Functions

Water Vapor

Functions derived from data of Kuhn (1963) for path length (u in precipitation - cm).

	<i>Log u</i>
$\epsilon = 0.11288 \log (1 + 12.63 u) *$	≤ -4
$\epsilon = 0.104 \log (u) + .440$	≤ -3
$\epsilon = 0.121 \log (u) + .491$	≤ -1.5
$\epsilon = 0.146 \log (u) + .527$	≤ -1
$\epsilon = 0.161 \log (u) + .542$	≤ 0
$\epsilon = 0.136 \log (u) + .542$	> 0

Carbon Dioxide

Presented by Shekhter and revised by Kondrat'yev (1969) (u_c in atm/cm).

$$\tau_c = \exp(-.3919 u_c^{.4})$$

* Presented by Zdunkowski and Johnson (1965).

C.3.2 Downward Infrared Radiative Flux

Computations for the downward infrared radiative flux are performed for m levels starting at the surface. The initial computation at each level m is to determine the first cloud level above level n at which a non-zero cloud amount occurs, and this level is saved.

The following values are initialized as:

$$\tau(m,m) = 1 \quad C(1a)$$

$$\epsilon_c = 1 \quad C(1b)$$

$$\epsilon_{a_m} = 1 \quad c(1c)$$

$$R_{\downarrow} = 0 \quad c(1d)$$

$$R_c = 0 \quad c(1e)$$

Then for a given level m , all layers above m to the top of the atmosphere ($n = n_g - 1$) will be used sequentially to compute the downward radiation at the level m . Therefore, the following computations are repeated for each level n until $n = n_g$ starting with $n = m+1$. It should also be noted in the following equations where the same term appears on both sides of an equal (=) sign that "=" does not mean equal but means "is replaced by" as is standard in FORTRAN programming.

The optical path length for aerosols is computed from

$$u_{a_m} = \sum_{i=m}^{n-1} \Delta u_a \quad c(2)$$

If a cloud base exists at level $n-1$, then

$$R_c = R_c + \sigma T_n^4 \epsilon_l \epsilon_c (\epsilon_a)_{n-1} \quad c(3)$$

where ϵ_l is the amount of cloud for layer l . Then

$$\epsilon_c = \epsilon_c (1 - \epsilon_l)$$

and the l is then incremented by 1 for the next cloud level, if any.

Then the transmission is computed using values of the transmissivity index or

$$\tau_{n,m} = e^{-1.6\kappa(u_a)_m} \tau_{(n,m)} \quad c(4)$$

Then, $R_{\downarrow}$ is incremented by

$$R_{\downarrow} = R_{\downarrow} + \sigma \left(\frac{T_n + T_{n-1}}{2} \right)^4 \epsilon_c \epsilon_a$$

$$\epsilon_a = \tau_{n-1,m} - \tau_{n,m} \quad C(5)$$

All computations from C(2) to C(5) are repeated until $n = n_s$. Then the downward flux at level m is computed from

$$R_{a+}(z_n) = R_{\uparrow} + R_{c\uparrow}$$

The result is stored. Then m is incremented by 1, and the computations are repeated from eqs. C(1a-e).

C.3.3 Upward Infrared Radiation

For each level $m > 1$, the following variables are initialized as

$$\tau_{m,m} = 1 \quad C(6a)$$

$$\epsilon_c = 1 \quad C(6b)$$

$$\epsilon_a = 1 \quad C(6c)$$

$$R_{\uparrow} = 0 \quad C(6d)$$

$$R_{c\uparrow} = 0 \quad C(6e)$$

Then for each level n starting with $n = m-1$ and ending with $n = 1$, the following procedure is used.

Find the first cloud base at a level $n < m$ and set l , if any are found. Then, if the cloud base is at level n , compute

$$R_{c\uparrow} = R_{c\uparrow} + \epsilon_l \sigma T_n^4 \epsilon_a \epsilon_c \quad C(7)$$

Then a new ϵ_c is computed as

$$\epsilon_c = \epsilon_c (1 - \epsilon_l)$$

and one is subtracted from l for the next lower layer of clouds.

The path length for aerosols is computed from

$$(u_a)_m = \sum_{i=n}^{m-1} (\Delta u_a)_m .$$

Then the transmissivity is computed from

$$\tau_{n,m} = e^{-1.66\kappa(u_a)_m} \tau_{(n,m)}$$

and

$$\epsilon_a = \tau_{n+1,m} - \tau_{n,m} .$$

Then

$$R_a^\uparrow = R_a^\uparrow + \sigma \left(\frac{T_n + T_{n+1}}{2} \right)^4 \epsilon_a \epsilon_c . \quad C(8)$$

Then n is decreased by 1, and, if $n > 0$, all equations from C(6a-e) through C(8) are repeated. If $n = 0$, the following is computed:

$$R_a^\uparrow(z_m) = R_a^\uparrow + R_c^\uparrow + \tau_{1,m} \epsilon_c \sigma T_I^4 . \quad C(9)$$

Then, the procedure is repeated for all levels m starting with eqs. C(6a-e).

C.3.4 Infrared Radiative Cooling Rate

The infrared cooling rates are computed for each layer when three or more levels have $R^\uparrow(z)$ and $R^\downarrow(z)$ computed. Then the cooling rates are interpolated from layered cooling rates to m levels.

The net flux $F_n(z)$ is computed for each level from

$$F_n(z_i) = R_a^\uparrow(z_i) - R_a^\downarrow(z_i) ; \quad 2 \leq i \leq N .$$

The cooling rates for the layer are computed for layer i , $i \geq 3$,

$$\left(\frac{\partial T}{\partial t}\right)_1 = \frac{g}{c_p \times 10^3} \left(\frac{F_n(z_1) - F_n(z_{1-1})}{P_1 - P_{1-1}} \right)$$

For level 2, the first level above the interface,

$$(S_1)_2 = \left(\frac{\partial T}{\partial t}\right)_2$$

For levels of $i > 2$, the cooling rates are computed from

$$(S_1)_i = \frac{P_i - P_{i-1}}{P_{i+1} - P_{i-1}} \left[\left(\frac{\partial T}{\partial t}\right)_{i+1} - \left(\frac{\partial T}{\partial t}\right)_i + \left(\frac{\partial T}{\partial t}\right)_1 \right] \quad c(10)$$

Storage will be saved if F_n and $\partial T / \partial t$ are saved for only levels and layers of $i+1$ and i .

C.4 SOLAR RADIATION

C.4.1 Downward Solar Radiation

The downward solar radiation is based on methods developed by Kondrat'yev (1969), McDonald (1960), Manabe and Strickler (1964), and Atwater (1970).

Compute the cosine of the zenith angle from

$$\cos Z = \sin \delta \sin \phi + \cos \delta \cos \phi \cos h$$

If $\cos Z \leq 0$, the sun is on or below the horizon. Therefore, in this case,

$$R_s + (z_1) = 0,$$

$$(S_2)_i = 0,$$

$$a = 1,$$

where $1 \leq i \leq m$, and no further computations for solar radiation are made.

Because of numerical problems as $\cos Z \rightarrow 0$, a lower limit is set on

$\cos Z$ and the radiation is reduced by a fraction, V , defined as follows:

$$V = 1,$$

and $\cos Z$ is unchanged if $\cos Z \geq 0.17365$;

$$V = \frac{\cos Z}{0.17365}$$

and $\cos Z$ is set to 0.17365 if $\cos Z < 0.17365$.

The initial flux for a horizontal surface at the top of the atmosphere is computed from

$$c_v = VI_0 \cos Z.$$

The flux is then reduced by clouds and aerosols above level N .

The solar optical path length is computed from

$$M = \frac{p(z_1)}{1013 \cos Z}.$$

The transmission ψ is then computed for all cloud layers above level N with j being the first cloud layer above N using the equations given in Table C-2, and using the cloud type as specified on input. Then

$$T_{c_m} = \prod_{i=j}^{n_c} [1 - \epsilon_{\lambda_i} (1 - \psi_i)].$$

If $n_c < j$, $T_c = 1$. T_{c_m} is also the fraction of clear sky above level N .

For each level m , the following are computed. The path length for water vapor from level m is computed from

$$u_m = \sum_{i=m}^{n_s-1} \Delta u_{w_i}. \quad C(11)$$

TABLE C-2

Transmission equations for clouds.

Cloud type	Equation
1. Fog	* $\psi = 16.26 + 0.54 M$
2. St	$\psi = 26.84 - 1.01 M$
3. Sc	$\psi = 36.58 - 1.49 M$
4. Cu	$\psi = 36.58 - 1.49 M$
5. Cb	$\psi = 23.63 + 1.45 M$
6. As	$\psi = 41.30 - 0.14 M$
7. Ac	$\psi = 54.56 - 2.36 M$
8. Ci	$\psi = 87.17 - 1.79 M$
9. Cs	$\psi = 90.55 - 6.38 M$

* ψ is in percent.

For aerosols, the path length is

$$u_{am} = \sum_{i=m}^{n_a-1} \Delta u_{w_i}$$

Further, T_a and T_s are computed for the layers above level m by

$$T_{am} = e^{-B_a u_{am} / \cos Z},$$

and

$$T_{sm} = e^{-B_s u_{sm} / \cos Z}.$$

Then

$$A_m = T_{am} T_{sm} T_{cm}.$$

The downward flux at level m is computed starting at level N and ending at level 1. For each level m , the following procedure is repeated. First compute

$$\gamma = 1.041 - 0.16 \left[\frac{0.000949P(z_m) + .051}{\cos Z} \right]^{.5}$$

$$T_1 = .485 + .515 \gamma$$

$$T_2 = 0.077 \left[\frac{u_m}{\cos Z} \right]^{.5}$$

The values T_c , T_a , and T_s are computed for the region above the layer. Then the variables at level m are computed from

$$G_m = c_v T_1,$$

$$W_m = -c_v T_2,$$

and

$$F_m = A_{m+1} (G_m + W_m).$$

However, when m is equal to N , the variables A_{m+1} are the same as for level N . Then the flux at level N is given by

$$R_s(z_N) = F_m, \quad C(12)$$

and further computations repeat from eq. C(11) if $N > 1$ after one has been subtracted from m . If $N = 1$, the incoming interface flux has been computed in C(12), and no further computations are necessary for downward solar radiation.

For $N > 1$ and $m < N$, the computations proceed as follows. If a cloud base i is at level m , the new transmission for total clouds is computed from

$$T_{cm} = T_{cm+1} [1 - \epsilon_i (1 - \psi_i)]$$

where ψ_i is computed according to Table 2 for the cloud type i . If

there is no cloud base at level m ,

$$T_{c_m} = T_{c_{m+1}}.$$

Then compute

$$T_2 = F_m (1 - T_{c_{m+1}} + T_{c_m})$$

$$T_{a_m} = T_2 (1 - T_{s_{m+1}} + T_{s_m}). \quad C(13)$$

Then the downward flux at level m is computed as

$$R_s(z_m) = T_{a_m} (1 - T_{a_{m+1}} + T_{a_m}).$$

C.4.2 Solar Radiative Heating Rates

The basic assumption made is that only downward radiation flux will have an influence on radiative heating. The net flux absorbed in a given layer is

$$F_n(z_m) = A_{m+1} (W_{m+1} - W_m) + 0.1 F_m (T_{c_{m+1}} - T_{c_m}) \\ + T_{a_m} (T_{a_{m+1}} - T_{a_m})$$

and

$$\left(\frac{\partial T}{\partial z} \right)_m = \frac{g}{10^3 c_p} \left(\frac{F_n(z_m)}{p(z_{m+1}) - p(z_m)} \right).$$

For layers with $m \leq N - 2$, the radiative heating at the level $m+1$ is computed from

$$S_{2_{m+1}} = \left(\frac{\partial T}{\partial z} \right)_m + \left(\frac{p(z_{m+1}) - p(z_m)}{p(z_{m+2}) - p(z_m)} \right) \left[\left(\frac{\partial T}{\partial z} \right)_{m+1} - \left(\frac{\partial T}{\partial z} \right)_m \right].$$

C.4.3 Upward Solar Radiation

The basic assumptions included here are that:

- 1) The upward flux of solar radiation does not influence the radiative heating rates.
- 2) The upward flux is unaltered by the atmosphere.

The upward solar radiation is composed of a) the radiation reflected at the surface, and b) the radiation scattered upward by atmospheric levels below level N (if $N > 1$). The upward flux at the surface is computed from

$$R_s^+ = a R_s(0) \quad . \quad C(14)$$

The albedo is computed for oceanic conditions from results of Sverdrup et al. (1942) given by

$$a = -0.0139 + .0467 \tan Z$$

with limits given by

$$0.03 \leq a \leq 1.00 \quad .$$

The albedo for inland lakes uses data obtained by Nunez et al. (1971) and is dependent on the total cloud amount. The total cloud amount is given by

$$E = 1 - \prod_{i=1}^{n_c} (1 - \epsilon_i) \quad . \quad C(15)$$

When $E \leq 0.5$, the albedo is computed from

$$a = \frac{.045}{\cos Z} \quad , \quad a \leq 1.0 \quad .$$

When $E > 0.5$, the albedo is computed from

$$a = \frac{1}{2} \left(\frac{.045}{\cos Z} + .00462 Z \right) ; a \leq 1.0 .$$

Over land, the albedo is specified as an input item.

The upward radiation from layer m is computed from

$$\begin{aligned} \Delta R_s(z_m) = & A_{m+1} (G_{m+1} - G_m) + 0.9 F_m (T_{c_{m+1}} - T_{c_m}) \\ & + T_{a_m} (T_{s_{m+1}} - T_{s_m}) . \end{aligned} \quad C (16)$$

The total upward solar radiation at level N is

$$R_s(z_N) = a R_s(0) + \sum_{n=1}^{N-1} \Delta R_s(z_n) .$$

C.5 TERRAIN EFFECTS ON RADIATION

The angle of the slope is computed from the input gradients of slope. The angle B is defined as the angle between the horizontal and the slope. It is also the angle between the normal to the slope and the zenith point. The angle B is computed from

$$B = \tan^{-1} \left\{ \left[\left(\frac{\partial H}{\partial x} \right)^2 + \left(\frac{\partial H}{\partial z} \right)^2 \right]^{\frac{1}{2}} \right\}$$

The azimuth of the slope η is computed from

$$\eta = \frac{3}{2}\pi - \tan^{-1} \frac{\partial H}{\partial z} .$$

If $\eta > 2\pi$, then subtract 2π from η for a corrected η . Compute the solar azimuth α from

$$\sin \alpha = \frac{-\cos \delta \sinh}{\cos Z}$$

and check to insure proper quadrant. Then the cosine of the incident angle is computed from

$$\cos i = \cos B \cos Z + \sin B \sin Z \cos(\alpha - \eta) .$$

The solar radiation is then modified to

$$R_s(0) = R_s(0) \frac{\cos i}{\cos Z} .$$

The effect on infrared radiation is then computed from

$$R_a^+(0) = R_a^+(0) \cos B .$$

C.6 REFERENCES

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Appendix D

The Non-Hydrostatic Model

The non-hydrostatic three-dimensional model differs only slightly from the hydrostatic model described in Section 2.0 of the report. This difference is manifested in the computation of the thermal wind. In the non-hydrostatic model the thermal wind equation is derived from the third equation of motion with the geostrophic assumption and the equation of state for an ideal gas. This derivation yields the equations

$$\begin{aligned}V_g(z) &= V_g(H) - \frac{g}{f \cdot T(z)} \int_z^H \frac{\partial T}{\partial x} dz + \frac{1}{f} \int_z^H \frac{\partial}{\partial x} \left(\frac{dw}{dt} \right) dz \\U_g(z) &= U_g(H) + \frac{g}{f \cdot T(z)} \int_z^H \frac{\partial T}{\partial y} dz - \frac{1}{f} \int_z^H \frac{\partial}{\partial y} \left(\frac{dw}{dt} \right) dz\end{aligned}$$

where $\partial T / \partial x$ and $\partial T / \partial y$ are computed according to equations (11) and (12) of main text [also, see equations (95a), (95b), and (95c) in Appendix A for the finite-difference form]. The above equations replace equations (9) and (10) (see Section 2.0 of the report). The essential difference between the two models in the computation of the thermal wind is in the addition of the second integral in the above equations. This term represents the horizontal gradient of the vertical acceleration.

In the finite-difference form the integrals are approximated through an application of the trapezoidal quadrature formula which was used in equations (94a) and (94b) of Section A.9.1 of Appendix A. The horizontal gradients of the vertical acceleration were approximated by spatially centered differences (see Section A.13.2).

Preliminary tests with the non-hydrostatic model revealed that on the coarse grid (~ 13 km) used in the Los Angeles simulations, the term involving the gradient

of the vertical acceleration would be approximately two orders of magnitude less than the term involving the temperature gradient, and, therefore, the differences between the hydrostatic and non-hydrostatic solutions would be small. Subsequent simulations on the Los Angeles coarse grid have revealed significant differences between the two models. We have attributed these differences to the topographic influence on the vertical acceleration. There have been comparisons of the solutions from the two models under identical input conditions. These comparisons have shown a tendency toward better temperature verifications but slightly worse pollution verifications. Our investigations with the non-hydrostatic model are continuing.

Appendix E

Advection Modifications

Numerical approximations to advection problems generally produce "numerical diffusion" of the solutions. This results from the uncertainty involved in attaching values to the dependent variables only at grid points. Thus, trajectories which do not pass directly from one grid point to the next do not explicitly define values of the dependent variables in regions where they are passing between grid points. This problem is resolved in Eulerian finite-difference schemes by various methods of interpolating or extrapolating results from points of explicit solution to off-trajectory points. Since the adequacy of an interpolation technique depends on distance between known points, the accuracy of interpolation (and thus the magnitude of the "numerical diffusion" effect) depends on the wind azimuth (see Figure E1), while for space- or time-variable winds the diffusion effect is also variable.

Numerical tests of the azimuthal effect were carried out. The results, reproduced in Figures E2 through E6, are presented in the form of concentration maps for emission from a single source in a steady, uniform windfield for each of several azimuths. It may be seen that for winds down the grid line, no diffusive effect is present, while for windfields with two finite vector components, every grid point in the quadrant downwind of the source receives some material. The steepness of the concentration ridge as well as the location and value of the concentration maxima vary with wind azimuth.

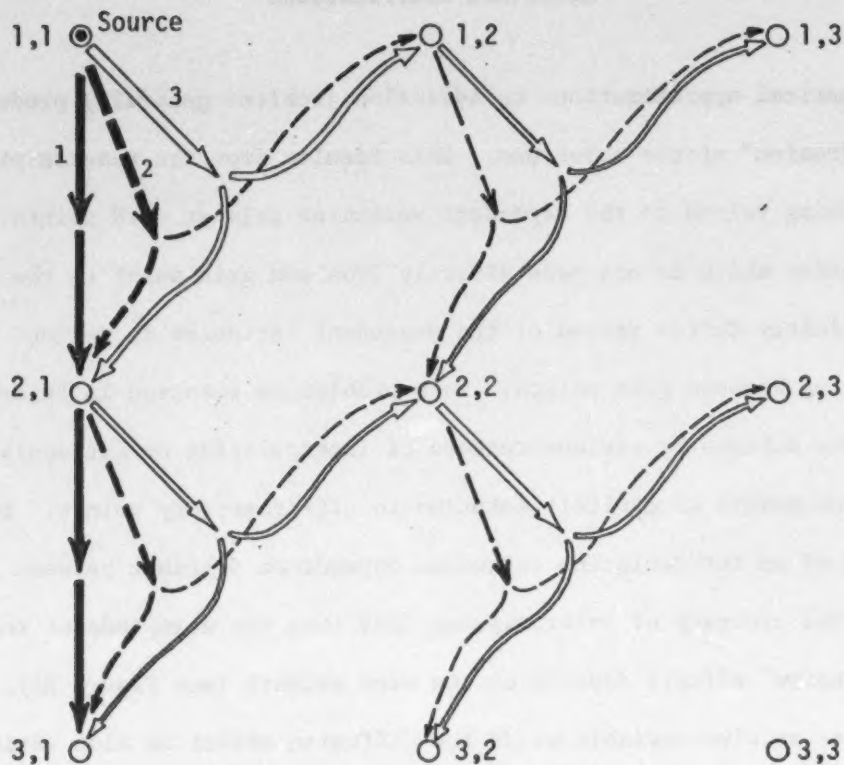


Fig. E1. Advective transfers for conventional Eulerian scheme with three wind trajectory azimuths.

- Trajectory 1: All material advected to point 2,1. Axial diffusion only. Point 2,1 is only source for further transfer. Material is confined to grid-line trajectory.
- Trajectory 2: Most material to point 2,1; some to point 1,2. Intermediate lateral diffusion. 2,1 and 1,2 become sources for further transfer. Material spreads to entire quadrant.
- Trajectory 3: Material evenly split between points 2,1 and 1,2. Maximum lateral diffusion 2,1 and 1,2 become sources for further transfer. Material spreads to entire quadrant.

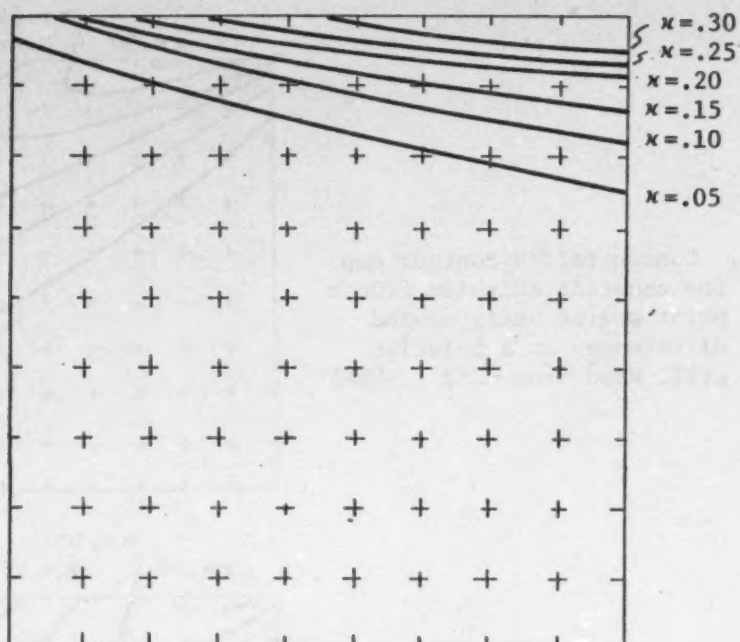


Fig. E2. Concentration contour map for constant emission from a point source using upwind differences on a Eulerian grid. Wind from $\sim 276^\circ$ ($\sim W$)

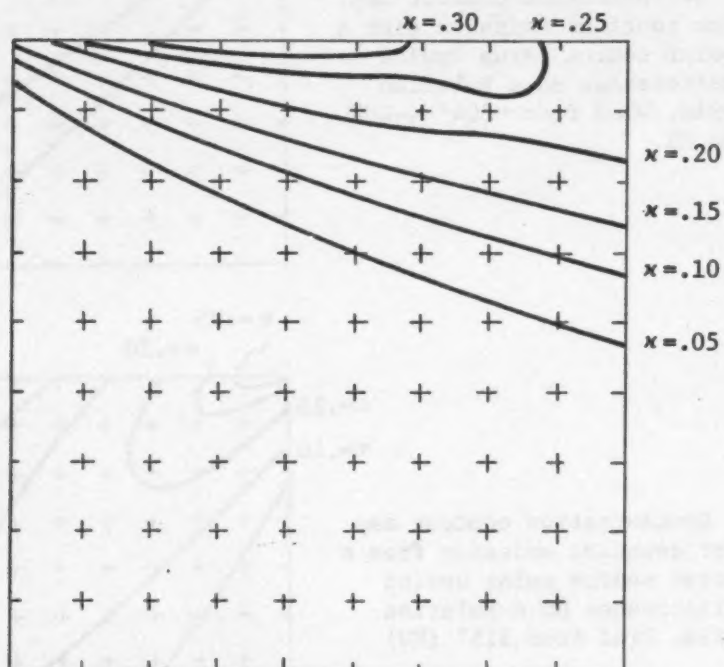


Fig. E3. Concentration contour map for constant emission from a point source using upwind differences on a Eulerian grid. Wind from $\sim 284^\circ$ ($\sim WNW$ by W)

Fig. E4. Concentration contour map for constant emission from a point source using upwind differences on a Eulerian grid. Wind from $\sim 293^\circ$ ($\sim$ WNW)

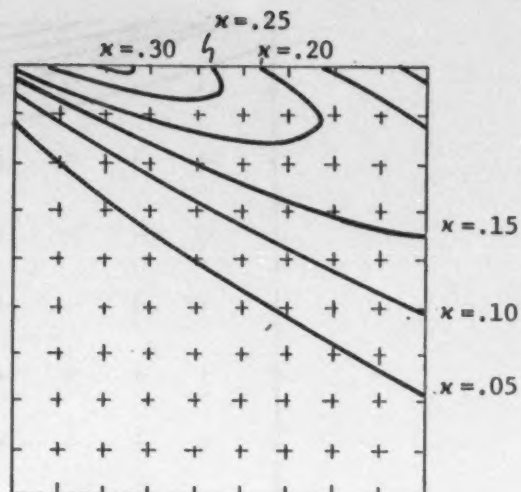


Fig. E5. Concentration contour map for constant emission from a point source using upwind differences on a Eulerian grid. Wind from $\sim 304^\circ$ ($\sim$ WNW by N)

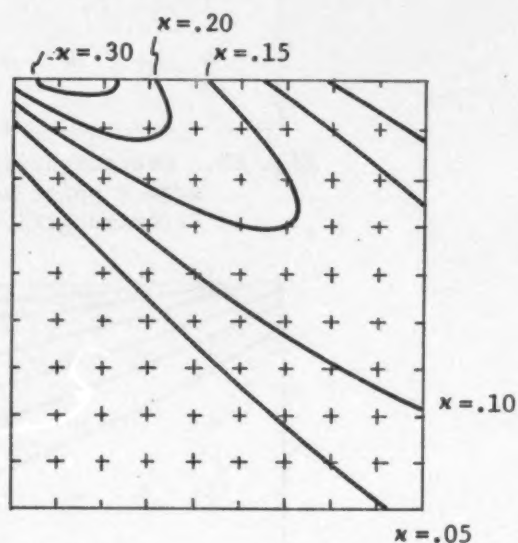
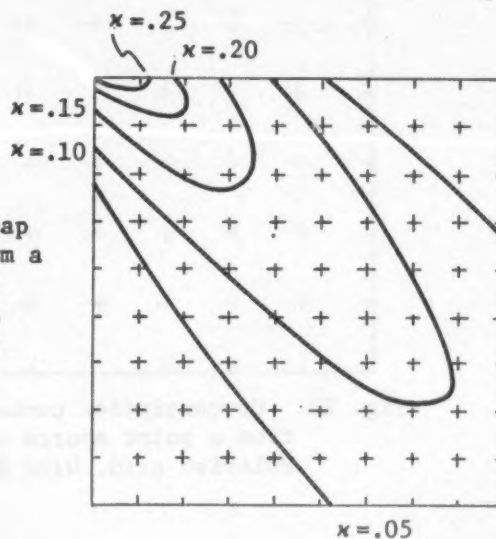


Fig. E6. Concentration contour map for constant emission from a point source using upwind differences on a Eulerian grid. Wind from 315° (NW)



E.1 Eulerian Modifications

Several techniques for minimizing these effects have been examined. One Eulerian technique appears plausible but has not been programmed for trial. In this scheme, the only change from conventional finite-differencing techniques would be in allowing advective transfers between diagonally neighboring points as well as along grid lines. That is, convective (presumably upwind, for stability) differences could be taken with one or all grid indices incremented by one or more steps. As shown in Figure E6, if one-cell diagonal transfers are allowed, numerical diffusion can be reduced so as to contain material within one half of a quadrant. If transfers are allowed across two-grid cells, as shown in Figure E8, the spreading can be reduced to a $2\pi/16$ sector ($22\frac{1}{2}^\circ$).

If it is assumed that winds cannot be defined to closer than a 16-point compass, the Eulerian scheme can be modified further to completely eliminate numerical spreading of an advected plume by allowing finite-difference transfers to only the single downwind neighbor that lies closest to the actual trajectory (see Figure E9). This will tend to preserve the concentration magnitudes to be expected downwind and would allow the explicit inclusion of correct lateral diffusion but would give somewhat less precise definition of the trajectory and thus of the locations of downwind maxima.

Such Eulerian schemes have equal or greater computing efficiency than conventional schemes in terms of the actual integration additions required, but would require considerable additional logical control steps. Time estimates have not been made.

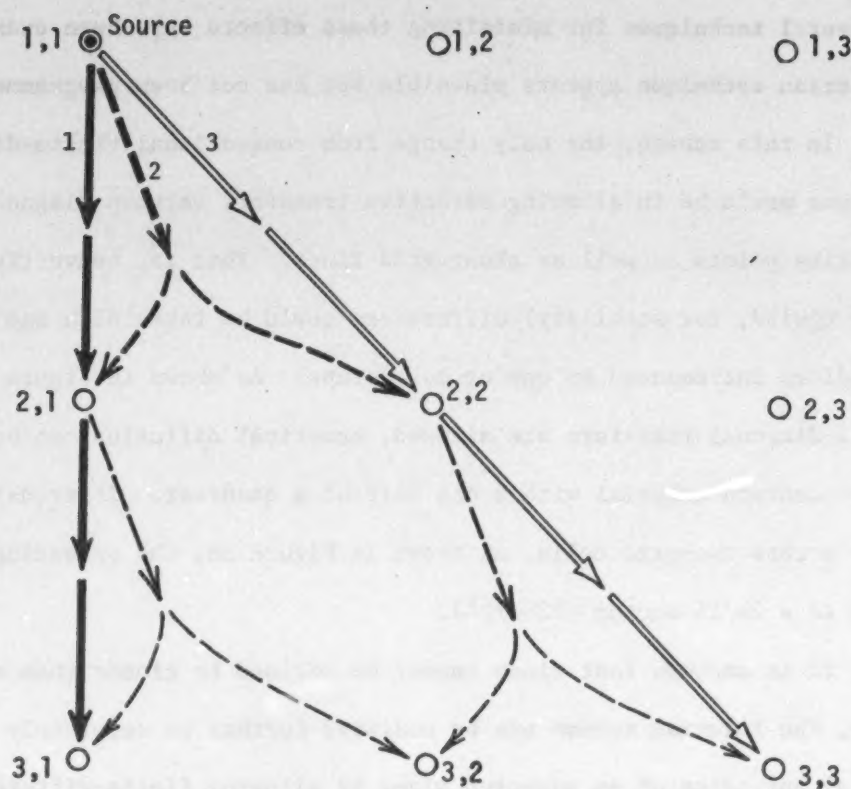


Fig. E7. Advective transfers for modified Eulerian scheme allowing transfers to diagonal neighbors. Three wind trajectory azimuths shown.

- Trajectory 1: All material advected to point 2,1. Axial diffusion only. Point 2,1 is only source for further transfers. Material is confined to grid-line trajectory.
- Trajectory 2: Material split between points 2,1 and 2,2. Maximum lateral diffusion. Points 2,1 and 2,2 become sources for further transfer. Material spreads through 45° sector.
- Trajectory 3: All material advected to point 2,2 axial diffusion only. Point 2,2 is only source for further transfer. Material is confined to diagonal trajectory.

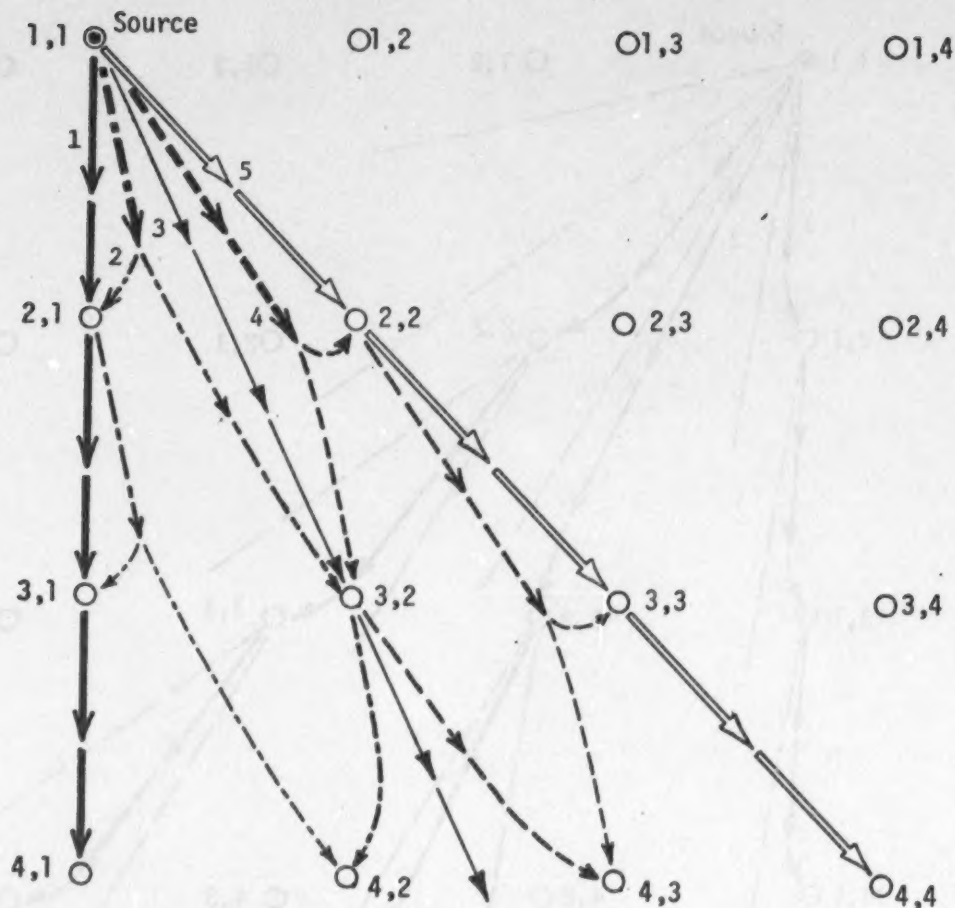


Fig. E8. Typical allowable advective transfers for a 16-point (two-cell) modified Eulerian scheme. Five wind trajectory azimuths shown.

Trajectory 1: As in Figs E1 and E7.

Trajectory 2: Material split between points 2,1 and 3,2 which become sources for further transfers. Material confined to $22\frac{1}{2}^\circ$ sector.

Trajectory 3: All material advected to point 3,2 which becomes only source for further transfers. Axial diffusion only. Material confined to half-diagonal trajectory.

Trajectory 4: Analogous to trajectory 2. Material confined to $22\frac{1}{2}^\circ$ sector.

Trajectory 5: As in Fig E7.

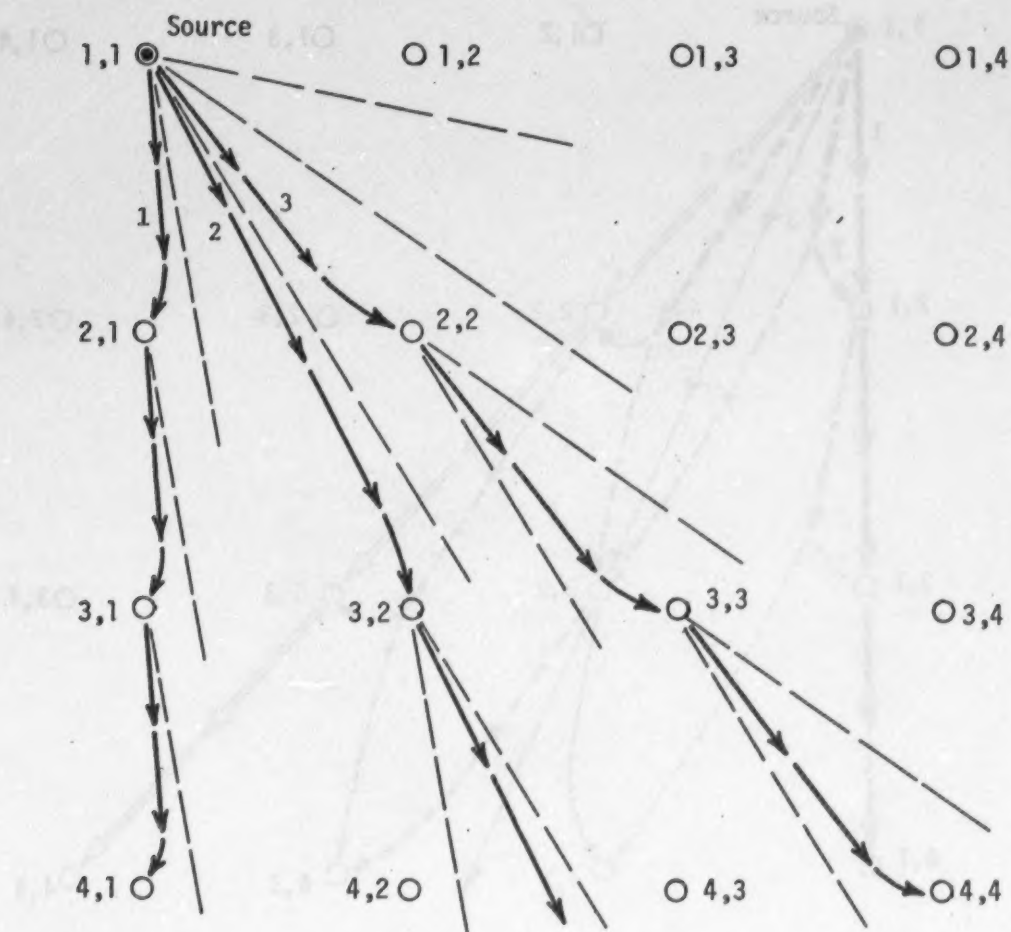


Fig. E9. Three typical trajectories in a 16-point nearest-grid-point Eulerian advection scheme.

E.2 Lagrangian Advection

Lagrangian particle-in-cell techniques are substantially free of numerical diffusion because positional resolution of advected material depends on the numerical accuracy (significant figures remaining) maintained in the computations and not on the grid definition.

Since we are concerned with the solution of a coupled set of differential equations, and since advection is a significant or even dominant effect for each dependent variable, a generalized Lagrangian scheme was developed and tested that

- allows different resolution schemes for each dependent variable (resolution is basically determined by the definition of the sources; and mass, momentum and energy sources, or sinks, are defined on scales consistent with available data and expected influence on resultant fields);
- is compatible with Eulerian techniques for treating explicitly included three-dimensional diffusion terms;
- substantially eliminates numerical diffusion; and
- is easily programmable.

The computer algorithm was developed by treating the conservation equations in the general form

$$\frac{dx_i}{dt} = \psi'(x_j) + \nabla \cdot K_i \nabla \psi'(x_j) \quad E(1)$$

where d/dt is the total (substantial, or convective) derivative; x_i is the i (th) conserved quantity; ψ' is a source term, a function of space or time that may depend on x_i and/or x_j (i.e., x_j 's are other dependent variables); K_i is a three-dimensional diffusion coefficient for i (th) variable, and ∇ is the gradient operator.

Integrated, in finite-difference form, we have

$$\chi_i^{n+1} = \chi_i^n + \psi(\chi_j^n) + \nabla \cdot K_i \nabla \psi(\chi_j^n) \quad E(2)$$

where ψ equals $\psi' \Delta t$; and n is the time step index taken along a trajectory. That is, χ^n is the distribution of χ a time step ago when it was a space step upwind. Similarly, ψ^n is the source distribution then, etc. Since χ_i^n is, in turn, dependent on $\psi(\chi^{n-1})$, etc., the algorithm can be reduced to

$$\chi_i^{n+1} = \sum_{v=0}^n \psi^v + \sum_{v=0}^n \nabla \cdot K_i \nabla \left(\sum_{\mu=0}^v \psi^\mu \right) \quad E(3)$$

so that χ at any time is the sum of "emissions" from one step upwind one time step ago, plus the "emissions" two time steps ago from two steps upwind, etc.; ψ may consist of any number of terms including the diffusive term. The diffusive term is written separately, however, to indicate its explicit representation in the model.

In equation E(3), ψ becomes the inventory of sources for the pollution equation, E(1), the pressure gradient (geostrophic wind) and buoyancy terms for the momentum equations, the solar and infrared heating for the temperature equation, E(1), etc. At each time step the diffusion term and the resultant χ fields are computed on an Eulerian grid, but the ψ , or "source", terms are accumulated as sets of advected points with the exact location of each "particle" computed. Since χ is eventually swept out of the field of interest (e.g., Connecticut SO_2 eventually moves out to the Atlantic), the ψ sets are screened to retain only "particles" of continuing interest. To avoid excessive recomputation of "particle" positions, the "particle" positions are noted relative to the current position of the first emitted "particle" from the same source. Interpolation is then involved in translating the advected cloud of particles onto the Eulerian,

fixed grid. This interpolation, which would produce numerical diffusion in some techniques does not accumulate positional error in the present techniques; thus, the only numerical diffusion present is that for a single (the latest) time step.

A different Lagrangian scheme (PICK) has been advanced for air pollution modelling (see ref. Sklarew, et al., 1971 of main text). Differences between the present scheme and PICK are the following.

- The present scheme is presented as a general scheme applicable to coupled sets of differential equations. PICK was presented as a limited algorithm for the solution of an equation for advected mass.
- In the present scheme, the dependent variables are carried as continuous variables, not discretized as in PICK; thus, it has a significant advantage over PICK in computational efficiency and/or accuracy. In PICK, trajectories must be computed for each "particle", thus the problem is effectively carried out on a much finer grid than the answers are available on.
- Both systems carry location along the trajectories as a continuous variable, but the advective velocity is defined only at grid points in the present scheme, whereas it is pseudo-continuous (by interpolation) in PICK. There seems to be little advantage in the velocity interpolation since it is difficult to parameterize significant grid scale variability in the velocity as turbulence. In practice, windfields should be defined on grid scales such that the point-to-point variability is small.

Initial trials of this technique were limited to non-diffusive advection from a steady point source, to compare with the similar tests with the Eulerian technique discussed above. The first trials with the Lagrangian technique used linear interpolation to translate between the moving and the fixed grids. This proved to be highly non-conservative in the resultant field because the concentration peaks that occurred between fixed grid points were not represented anywhere; subsequent trials used nearest grid point translations, so that each particle in the Lagrangian set was assigned to a grid point in the resultant fixed grid.

These results are shown in Figures E10 through E12. It may be seen that the system is conservative and as non-diffusive as may be (trajectories at an angle to grid lines simply cannot be represented by a single straight line of points; there is necessarily a "staircase" effect). The concentrations do differ for different trajectory azimuths, however. This is because the linear density of a set of diagonally joined squares is less than that of a laterally joined set. Over a swath of two or three cells width, which is about all the resolution that can be expected from any grid solution, the mean concentrations are identical. It is important to note that this accentuates the difficulty of "verifying" any grid model output with point observations, even though the model may be more "correct" and/or relevant.

Further tests showed that circular (or spherical) arrays of sources give off plumes that have essentially no azimuthal variation of center-line concentration. Similarly, solutions for single source emissions resolved on a grid defined as a matrix of packed spheres give no azimuthal effect. It is not presently felt that this effect is important enough for dense arrays of sources (or pseudo-sources for momentum, energy, etc.) to warrant further experimentation.

Introduction of the Lagrangian advection scheme described above proceeded by stages. Because of the complexity of converting the full urban boundary layer model to the Lagrangian form, initial tests were carried out with the two-dimensional "Connecticut Model".

Several logical problems appeared and were solved. Some of the problems were compounded by the necessity, because of core space limitations, of treating the grids by successive segments. Some of these problems were the following:

Fig. E10. Concentration contour map for constant emission from a point source using Lagrangian advection scheme with nearest grid-point interpolation - fully conservative. Wind from 360° (N)

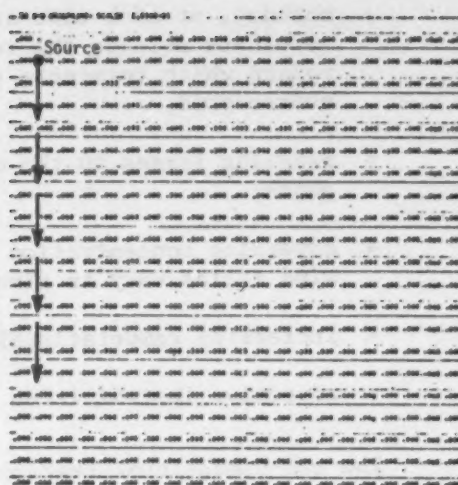


Fig. E11. Concentration contour map for constant emission from a point source using Lagrangian advection scheme with nearest grid-point interpolation - fully conservative. Wind from 337-1/2° (WNW)

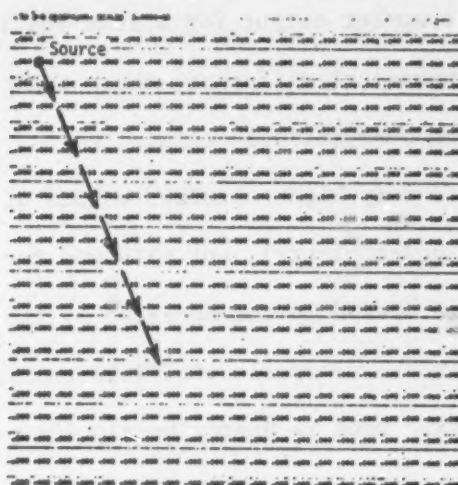
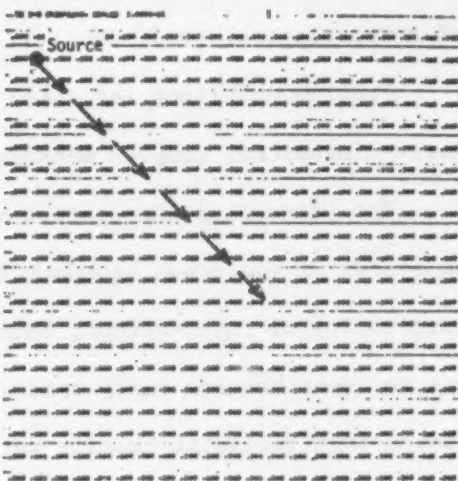


Fig. E12. Concentration contour map for constant emission from a point source using Lagrangian advection scheme with nearest grid-point interpolation - fully conservative. Wind from 315° (NW)



- masking, at each time step, the source points whose trajectories terminate outside the resultant grid as well as resultant grid points which terminate trajectories which originate outside the source grid;
- handling losses to the upper air in zones of horizontal convergence;
- advecting concentration fields as well as emission fields when wind fields vary in time;
- increasing computational efficiency; and
- advective instabilities introduced by vertical loss mechanism.

The two-dimensional Lagrangian model has been completed and tested. The computer output for a test run is presented in Figure E13. The horizontal numerical diffusion, characteristic of Eulerian schemes, has been found to be substantially eliminated as expected. The absence of such diffusion led to very high pollutant values at grid squares with very large point sources (power plants), but this was reduced to expected levels with the introduction of upward losses modelled by the thermally generated updrafts which are used in the mesoscale windfield analysis to compute horizontal winds. Computer time used is approximately 10m per second per grid point per time step with an additional 20 seconds for initial computations and 20 seconds per change of meteorological conditions.

Problem solutions for these two-dimensional tests are applicable to the three-dimensional coupled meteorology Lagrangian model.

The Lagrangian integration scheme for the complete set of differential equations of the urban boundary layer model was programmed in ANAL70. The programming of input-output, boundary conditions, and auxiliary equations was not done because early test runs with the operating Eulerian model showed that realistic results were obtainable in spite of the diffusive properties of the model. In fact, CO verifications were comparable to those

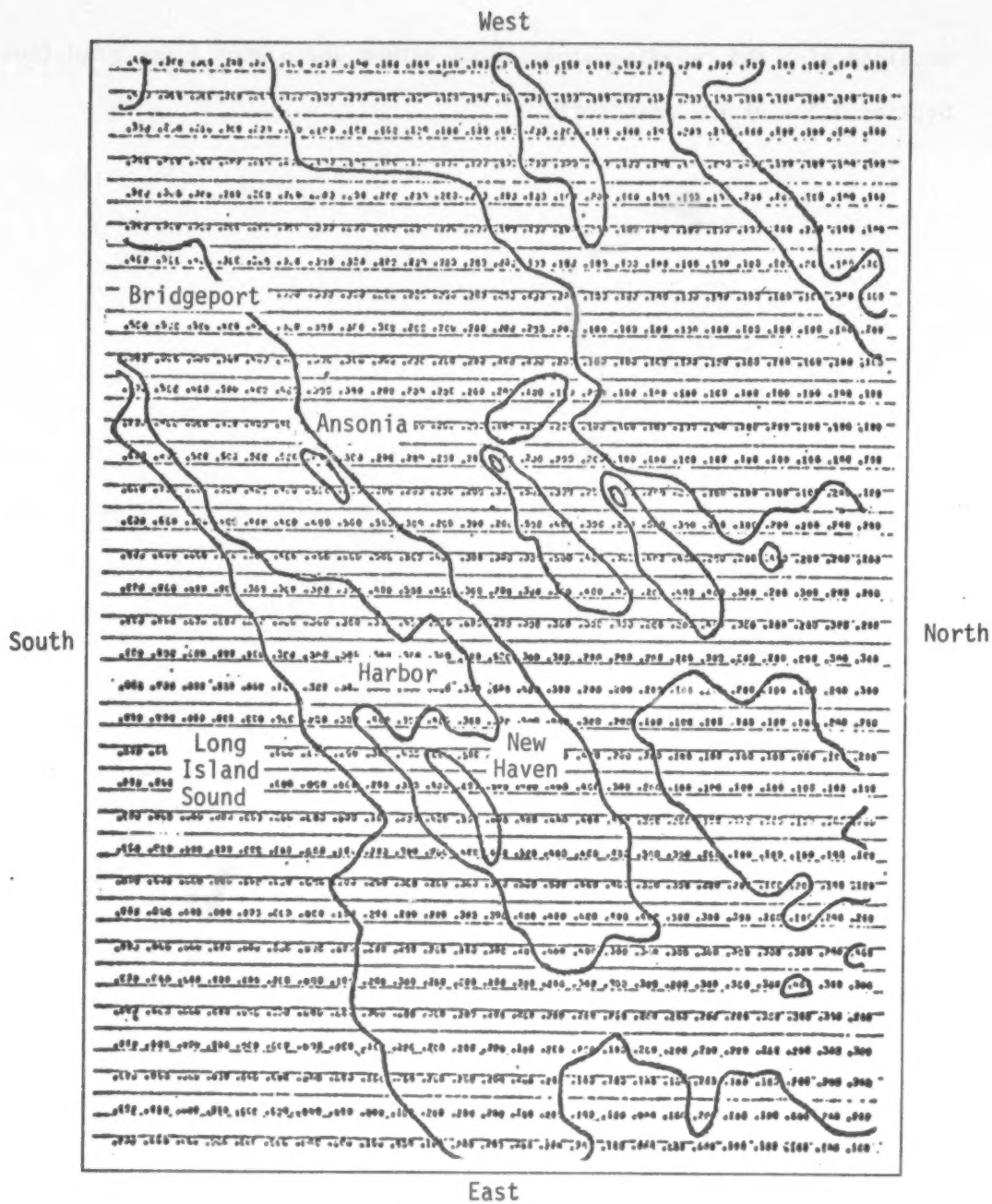


Fig. E13. Excerpt from computed concentration map showing South-Central Connecticut.

- Lagrangian Advection.
- Southwest wind (1 m/sec) veering to WSW.
- SO₂ emissions, January.
- 5000 ft grid spacing.
- Topographic and thermal wind disturbances.

obtained with the two-dimensional PICK method and a much finer grid (see Section 3.3.4 of the main text).

